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如何使用SciFinder获取科技信息

安徽师范大学

2016.09.13

SCIFINDER®
A CAS SOLUTION

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索 （ PatentPak ）
  - 物质检索
  - Markush检索
  - 反应检索（ MethodsNow Synthesis ）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

美国化学文摘社—Chemical Abstracts Service

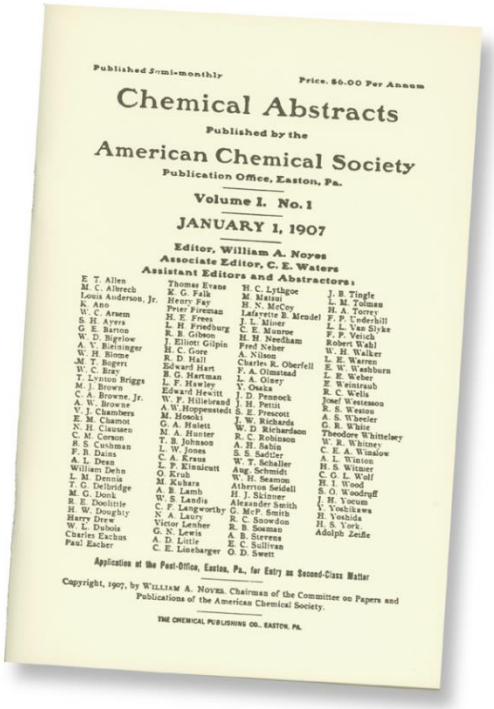
- ACS的分支机构
- 创建于1907年，简称”CAS”
- 最早创立了《化学文摘》
- 密切关注，索引和提炼着全球化学相关的文献和专利
- 总部座落于俄亥俄州的哥伦布市

SciFinder® A CAS SOLUTION

1907年，信息的汇集、管理发生了重大的变化

威廉•诺伊斯
(William A. Noyes)

- “化学文摘”创刊
- 当年编制近12,000条文摘
- 今天，CAS每年收录、创建来自期刊、专利和其他已公开信息的文摘达到了100余万条



Published Semi-monthly Price, $6.00 Per Annum

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Published by the

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Publication Office, Easton, Pa.

Volume I. No. 1

JANUARY 1, 1907

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Application at the Post-Office, Easton, Pa., for Entry as Second-Class Matter

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CAS——构建最高质量的化学数据库

arXiv.org

Aldrichimica Acta

ACS chemical biology

BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

division of polymer chemistry, inc American Chemical Society

JACS JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical Neuroscience

Cornell University Library

The Journal of Physical Chemistry Letters

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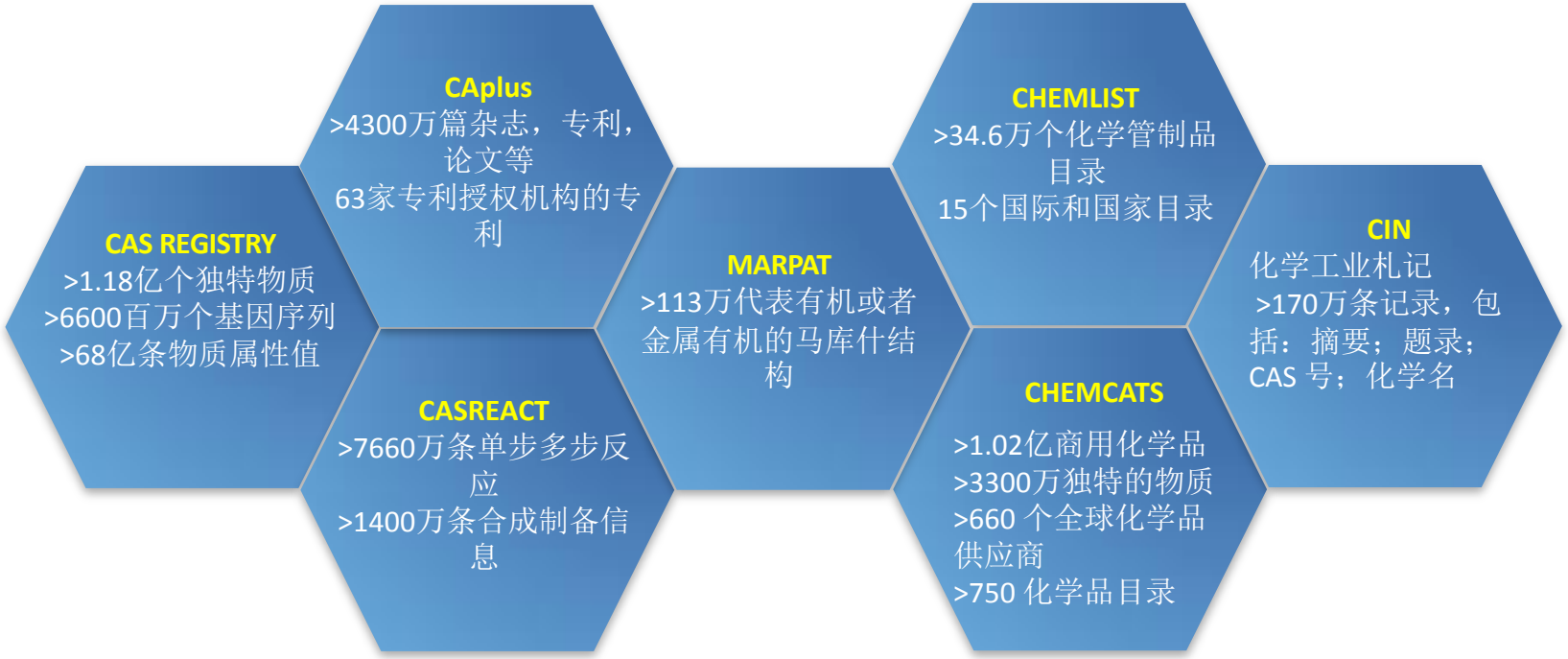

CAS数据库——源于化学，超越化学

生物化学：

农化产品管控信息,生化遗传学,发酵,免疫化学,药理学

有机化学各领域：

氨基酸,生物分子,碳水化合物,有机金属化合物,类固醇

大分子化学各领域：

纤维素、木质素、造纸;涂料、墨水
染料、有机颜料 ;合成橡胶 ;纺织品、纤维

应用化学各领域 ：

大气污染,陶瓷,精油、化妆品,化石燃料,黑色金属、合金

物理、无机、分析化学各领域：

表面化学,催化剂,相平衡,核现象,电化学

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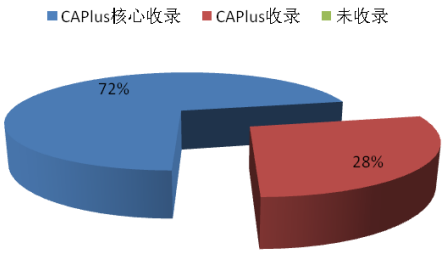
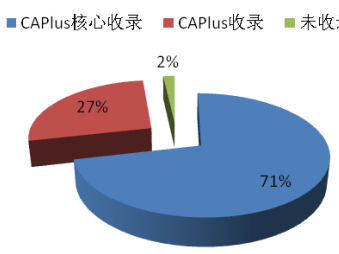
CAS对各学科期刊文献的收录（部分）

SciFinder收录材料学科期刊比例
（源自156份影响因子大于1的期刊）



SciFinder收录化学工程学科期刊比例
（源自56份被SCI收录的期刊）



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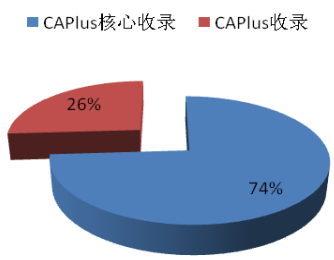
（源自50份被SCI收录的期刊）



SciFinder收录药学类期刊比例
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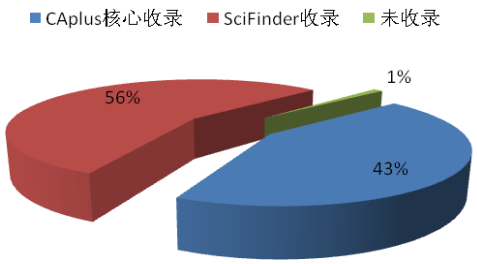
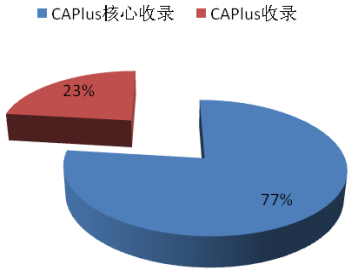


SciFinder收录生物化学类期刊比例
（源自26份被SCI收录的期刊）



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CAS数据库最具价值的内容——人工索引

4. Process for preparation of novel sofosbuvir crystal

By: Zhou, Haohui; Lin, Guoliang; Wu, Yao; Zou, Wenjuan; Chan, Yunxia
Assignee: Beijing Winsunny Pharmaceutical Co., Ltd., Peop. Rep. China

The invention relates to a novel sofosbuvir crystal having high stability and soly. The novel sofosbuvir crystal is prepd. through crystg. sofosbuvir in pos. solvent and neg. solvent. The method has high repeatability, easy control, high yield, and high product purity.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105732751 PATENTPAK	A		Jul 6, 2016	CN 2014-10742897	Dec 9, 2014

Priority Application

CN 2014-10742897	Dec 9, 2014

Indexing

Carbohydrates (Section33-9)

Section cross-reference(s): 34, 63

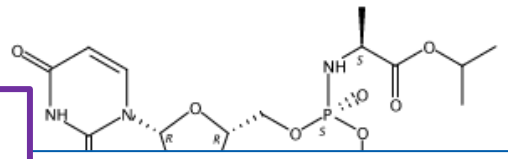
Concepts

Crystallization
Drug bioavailability
Hepatitis C
Hepatitis C virus
Homo sapiens
Human
Pharmaceutical coated tablets

Substances

1190307-88-0P Sofosbuvir
Absolute stereochemistry.

Page 2 in PATENTPAK



Tips:

1. 98%以上的文献，都经过人工索引
2. 用Index Term标引文献中的重要技术术语
3. 用CAS RN标引出文献中的重要物质
4. 用CAS Role标引文献中重要物质的研究领域

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CAS人工标引解决的问题

- 检索词的同义词拓展：解决不同科研人员由于教育背景、语言、表达习惯不同导致的对同一个技术术语描述的差异。
- 用名称、分子式等检索化合物，会导致检索不全、不准的问题。CAS RN很好的解决了该问题，帮助检索人员实现精准定位化合物的目标。
- 利用SciFinder中的标引信息（Index Term，CAS RN，CAS Role），提高效率，启发思路。

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CAS最新动向—解决方案

PatentPak™

NCI™ Global
A Solution Powered by CAS

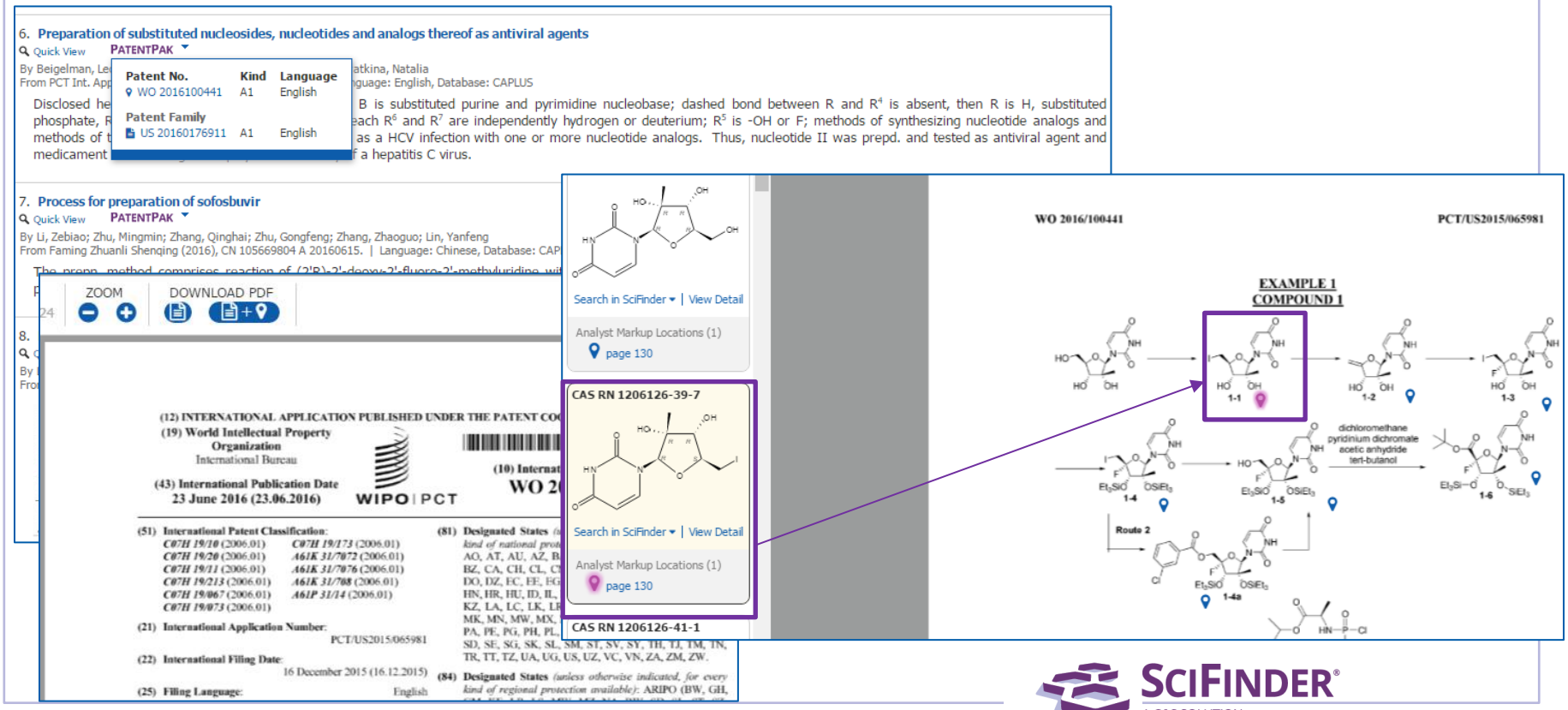
MethodsNow™
A CAS SOLUTION

ChemZent™
A CAS SOLUTION

SciFinder®
A CAS SOLUTION

CAS最新动向—解决方案

- CAS于2015年2月正式发布PatentPak™
- 专利工作流程解决方案
- 极大节约用户在研究专利时的时间
- 快速查找定位专利中的关键化学信息



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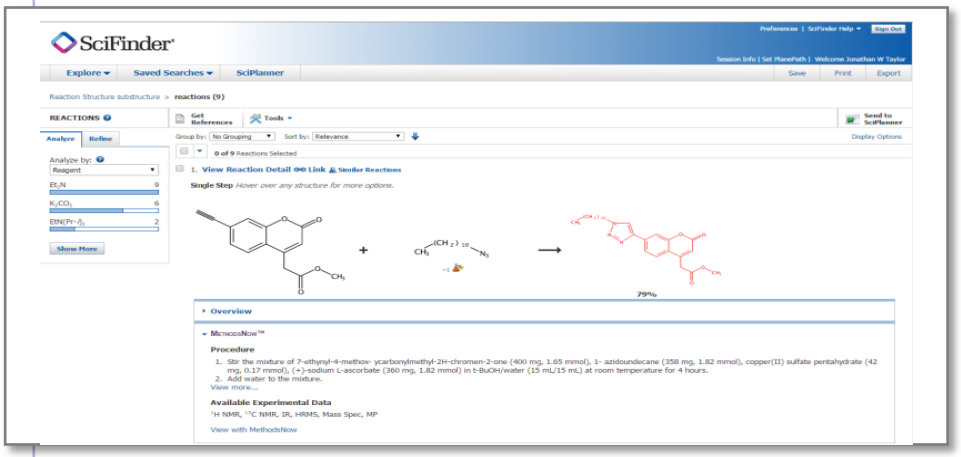
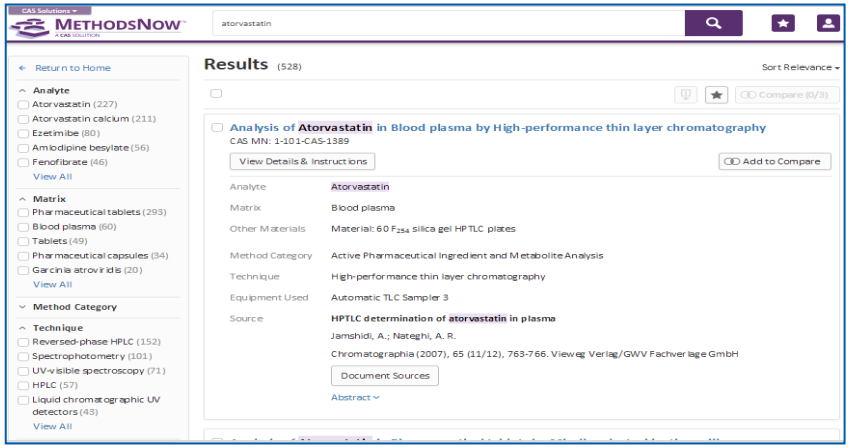
CAS最新动向—解决方案

- CAS于2016年2月正式发布MethodsNowTM
- 最大方法信息合集
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求



嵌在SciFinder中的合成模块



单独的分析界面

SCIFINDER®
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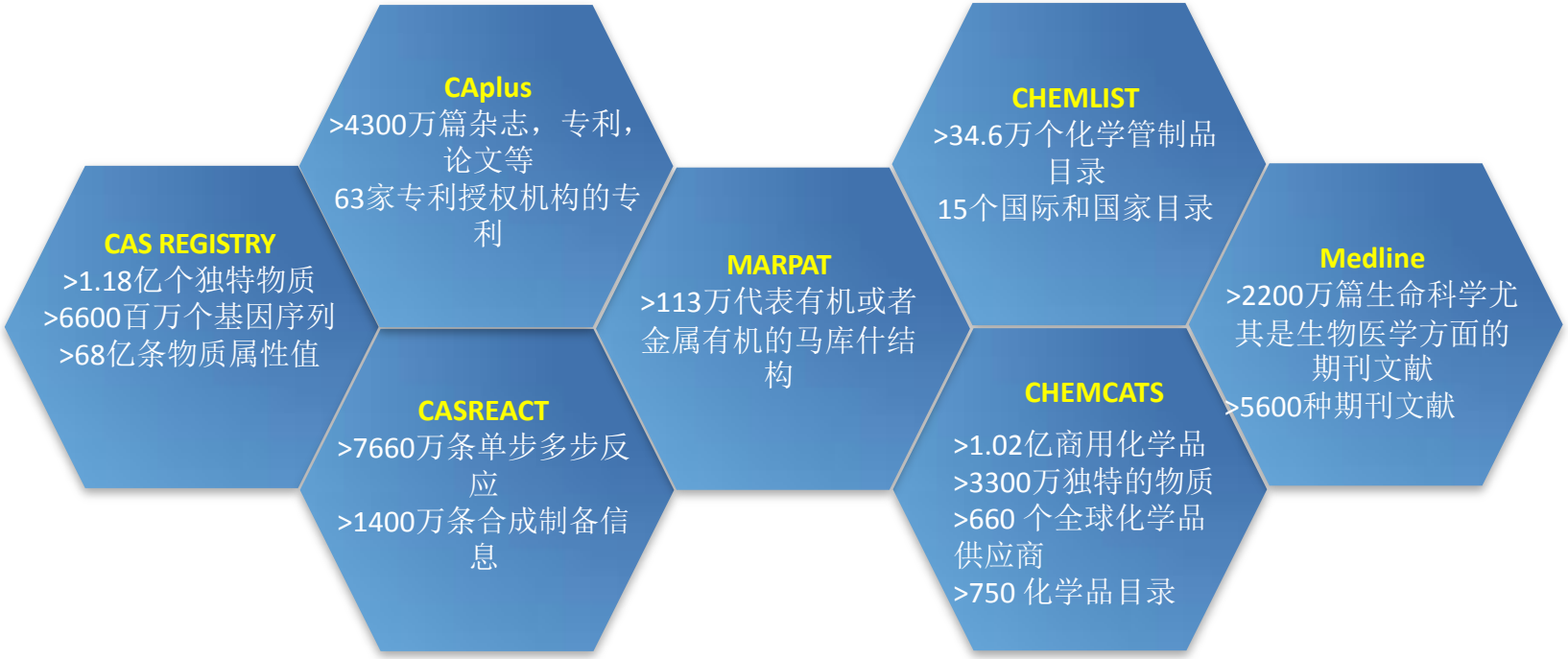
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SciFinder覆盖的数据库



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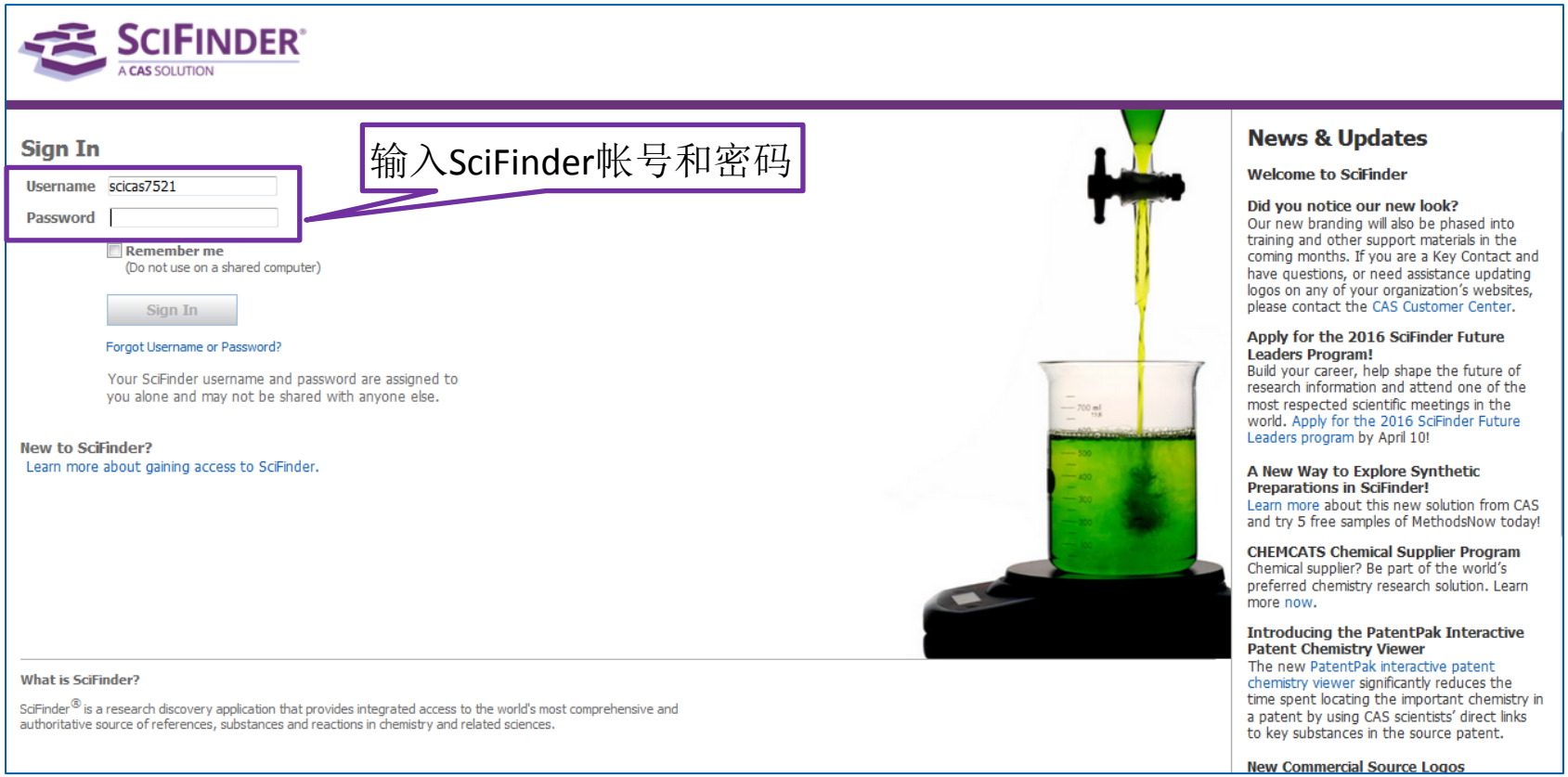
SciFinder登录网址: https://scifinder.cas.org/



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SciFinder主界面

SciFinder检索——文献检索

- 文献检索方法
  - 主题检索
  - 作者名检索
  - 机构名检索
  - 文献标识符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献

- 检索策略推荐
  - 关注某特定领域的文献：主题检索
  - 关注物质有关的文献：先获得物质，再获得文献
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索

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文献检索——主题

主题检索：纳米材料与基因的相互作用

检索式： Nanomaterial of gene

关键词之间用介词连接：in, with, of...

SciFinder
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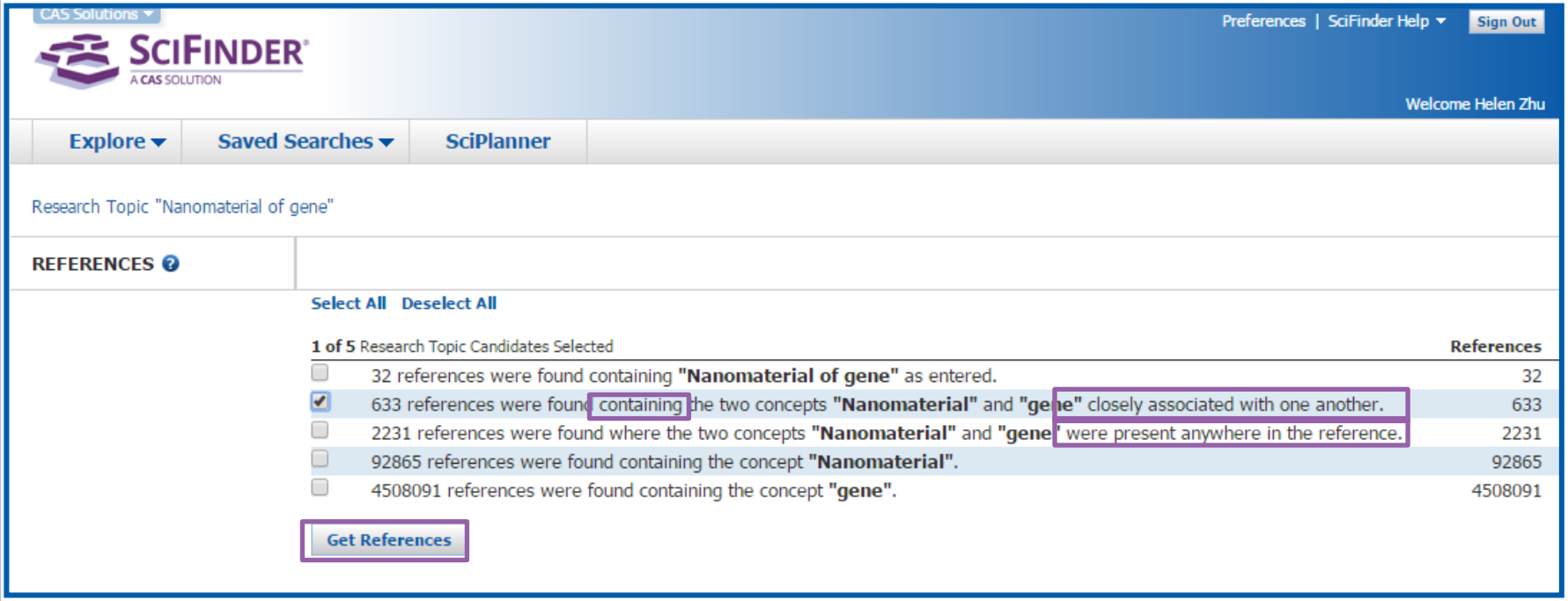
主题检索的候选项



"Concepts"表示对主题词做了同义词的扩展；

"Closely associated with one another"表示同时出现在一个句子中;

"were present anywhere in the reference"表示同时出现在一篇文献中；

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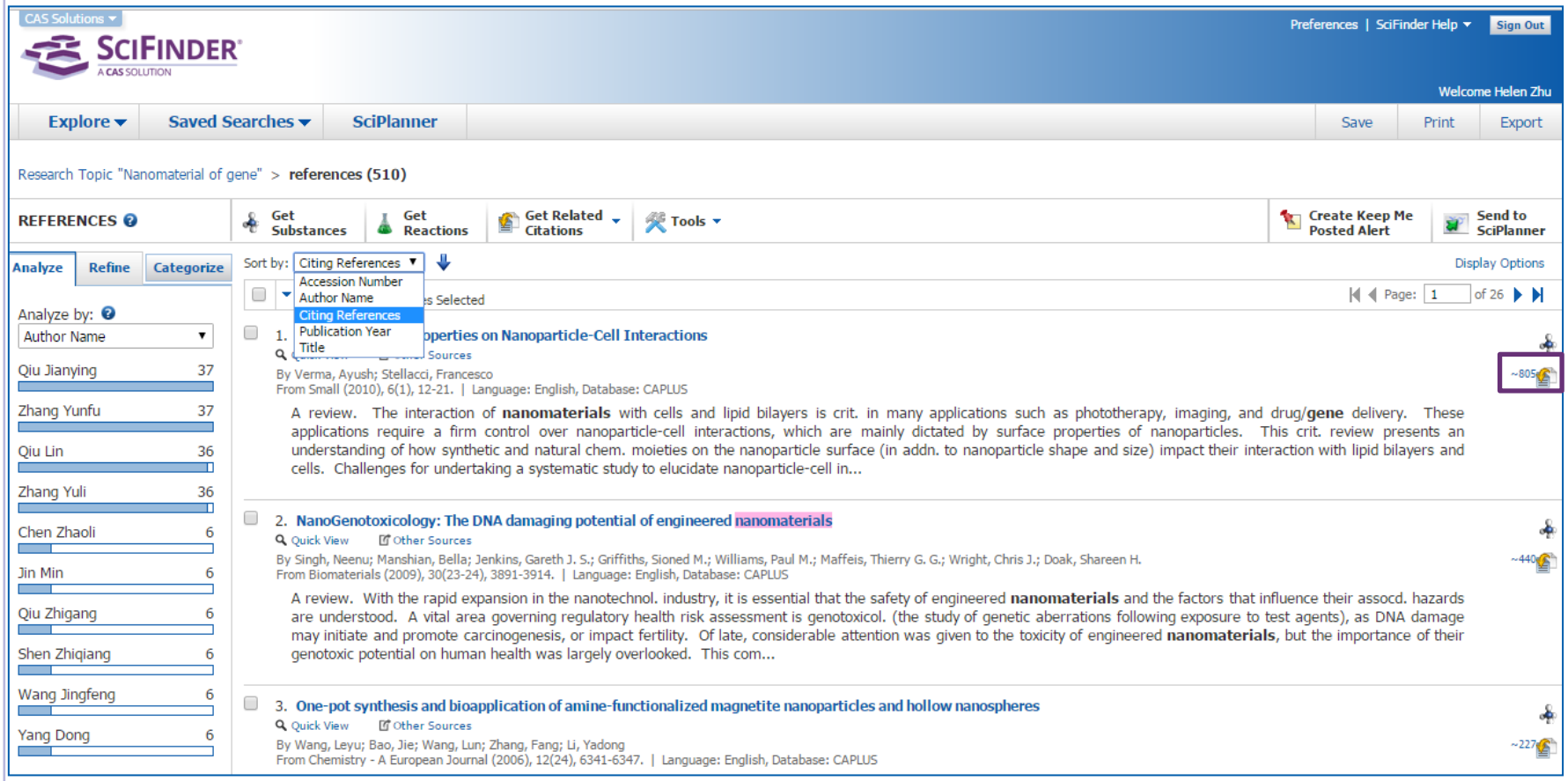
A CAS SOLUTION

按被引次数排序— Citing References



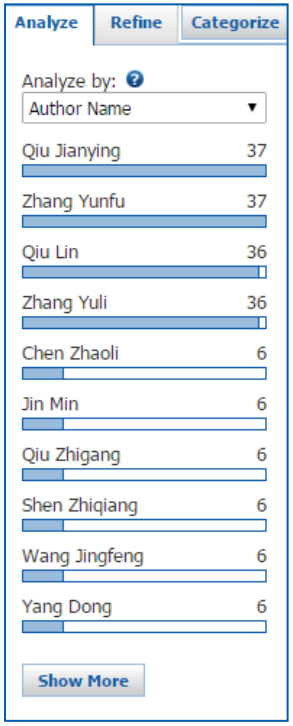
Citing Reference: 帮助找到最重要的文献

文献检索结果

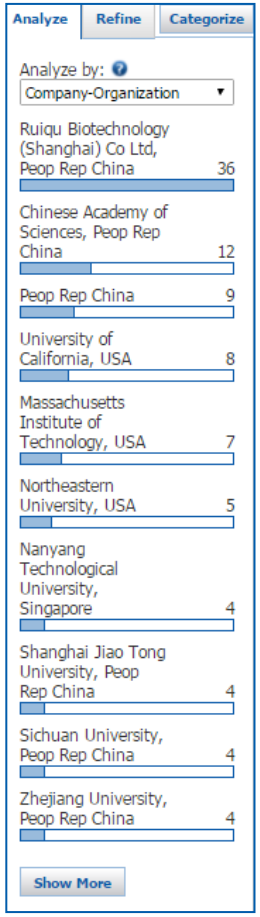
SciFinder提供强大的文献处理工具，帮助处理文献

文献检索结果的Analyze

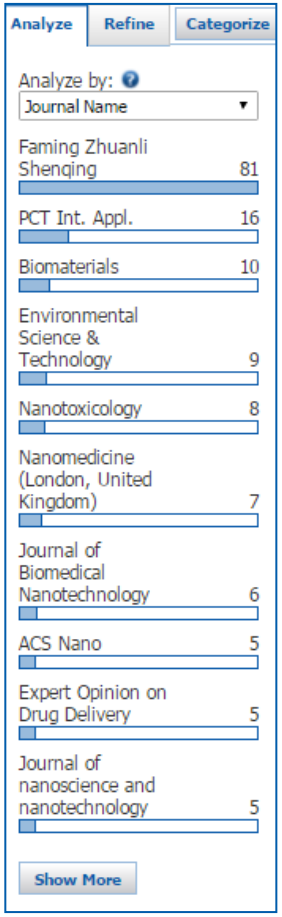
本领域研究人员



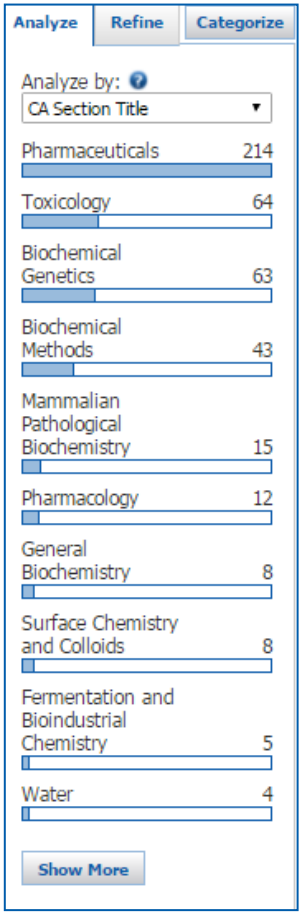
本领域研究机构、合作伙伴、竞争对手



期刊



涉及学科领域



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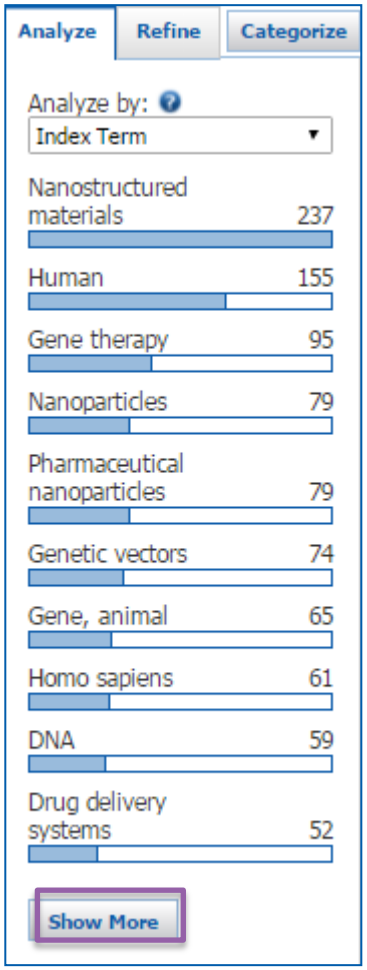
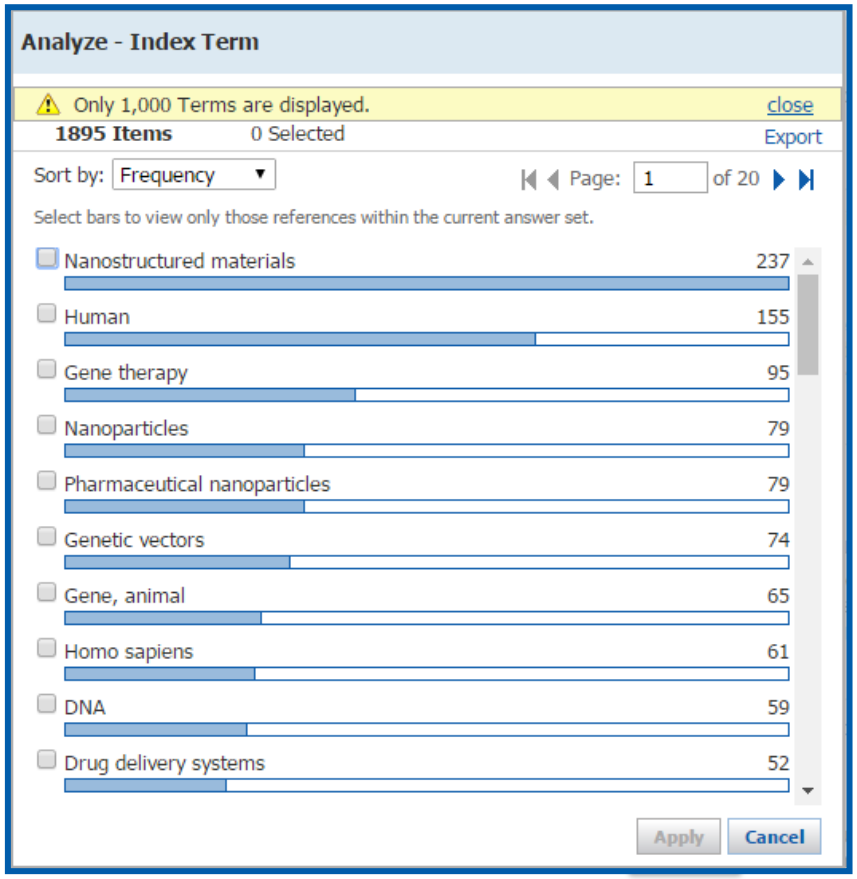
文献检索结果的Analyze



Index Term：

帮助用户了解涉及到的重要技术术语，并修正检索词



选择感兴趣的内容，点击Apply

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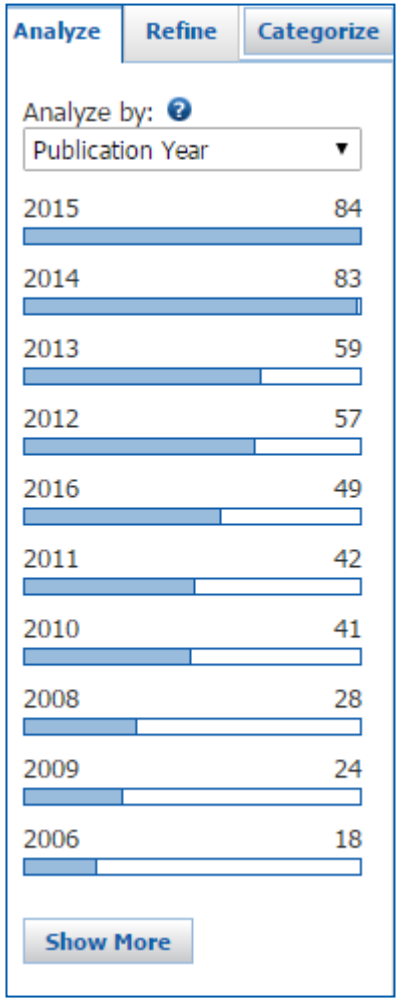
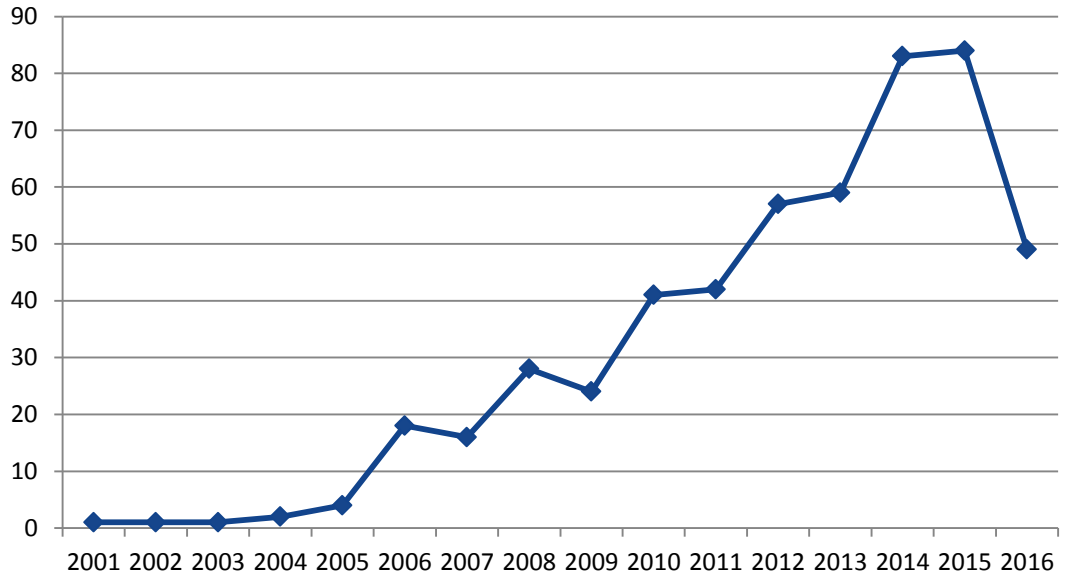
文献检索结果的Analyze





Publication Year: 分析领域发展趋势

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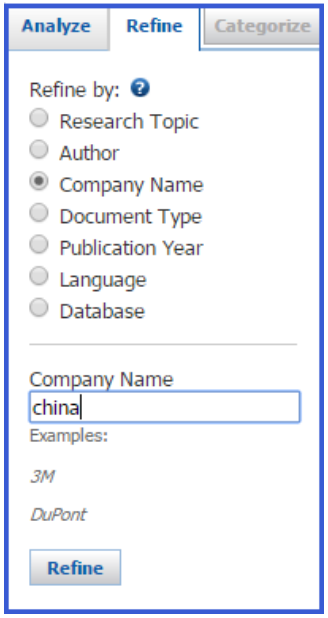
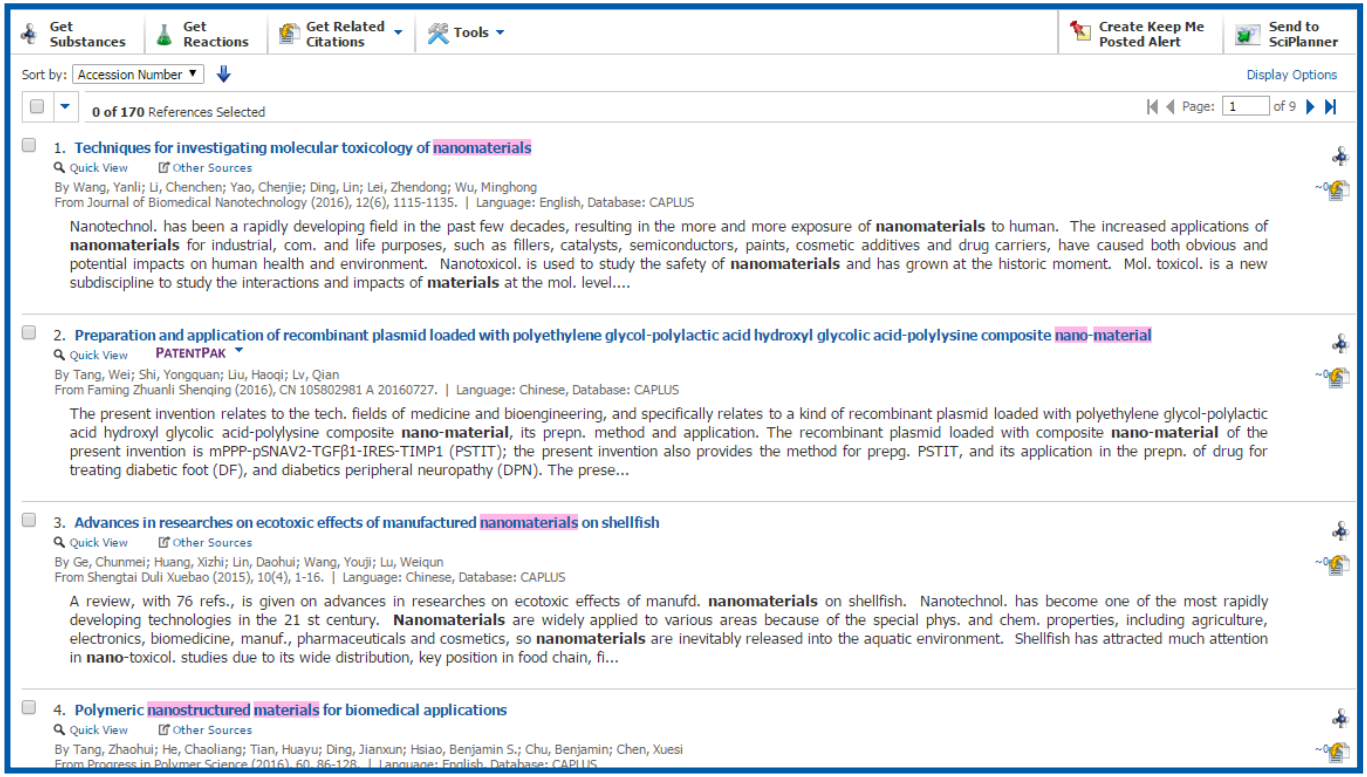
文献检索结果的Refine



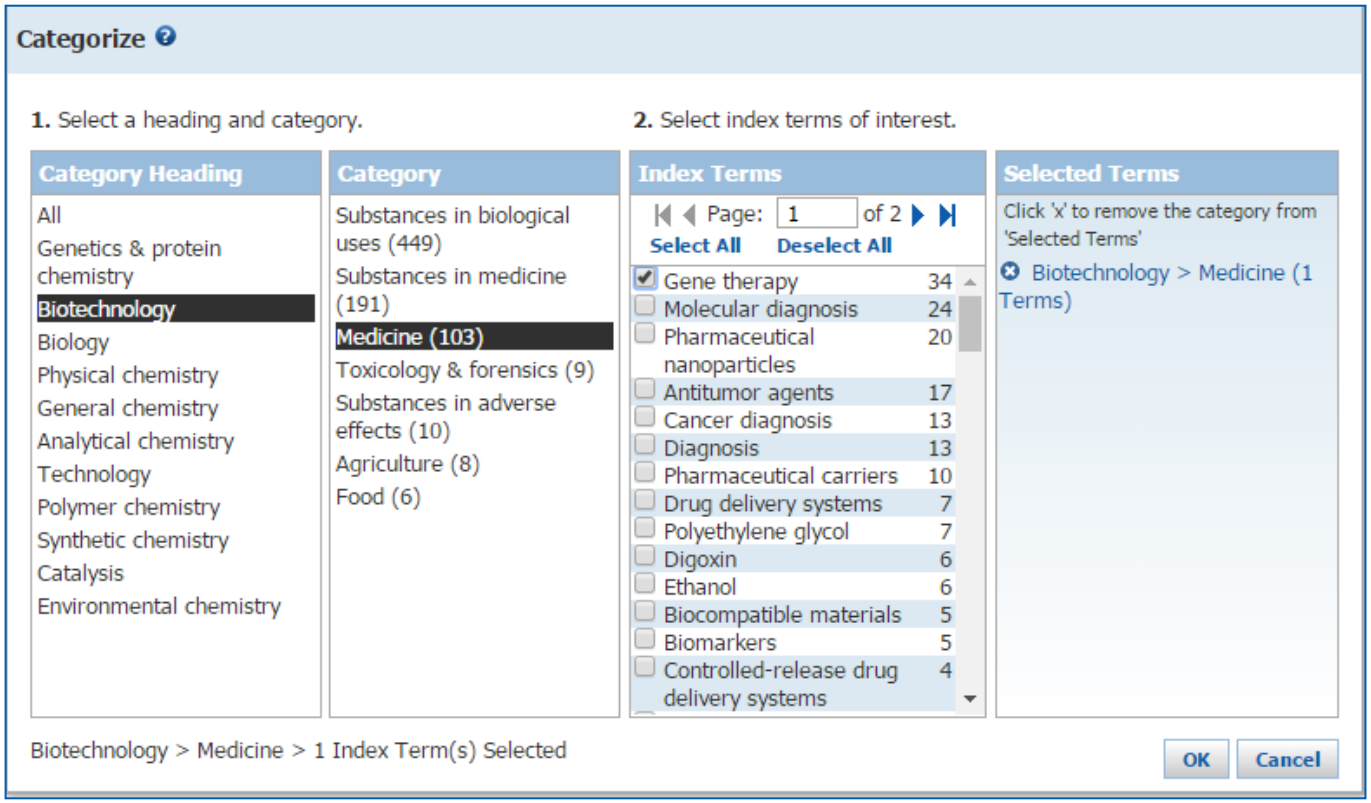


Refine：帮助用户迅速获得需要的文献

SciFinder® A CAS SOLUTION

文献检索结果的Categorize

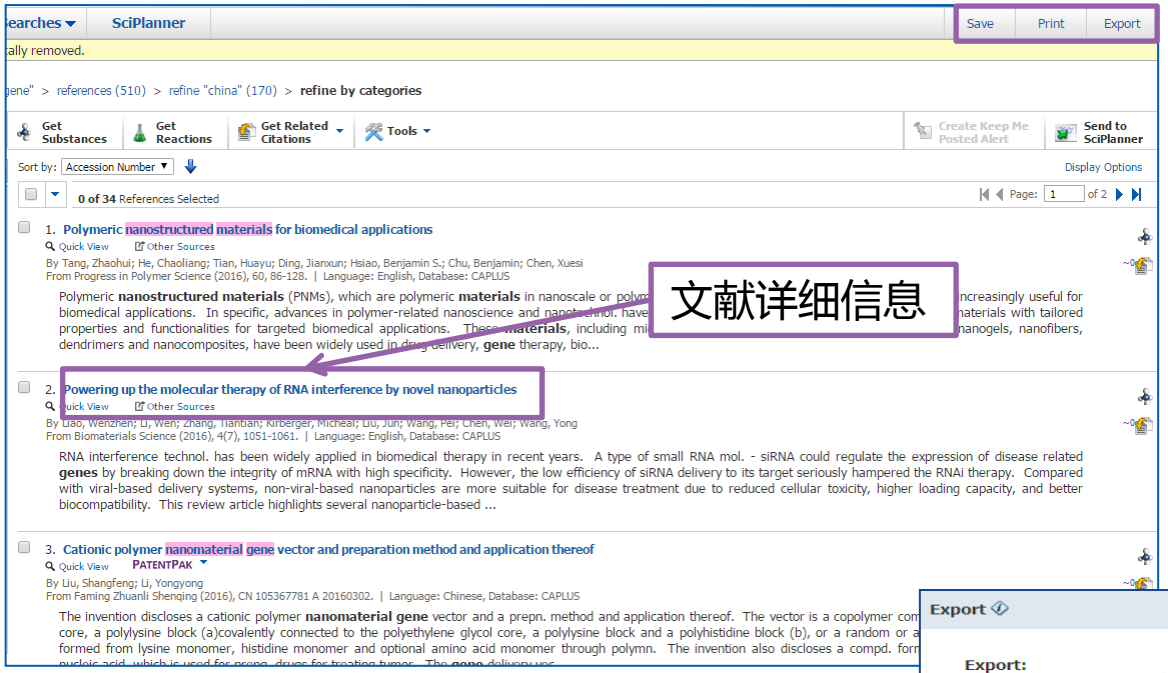
学科领域主分类　　学科领域副分类　　Index Term　　选中的Index Term



Categorize学科分类功能，基于Index Term，根据大学科方向对文献进行自动分类。

SciFinder® A CAS SOLUTION

结果集的保存— Save, Print, Export



Save：保存在服务器上，方便以后登陆查看，每次可存1万条记录。

Export：导出至本地电脑。

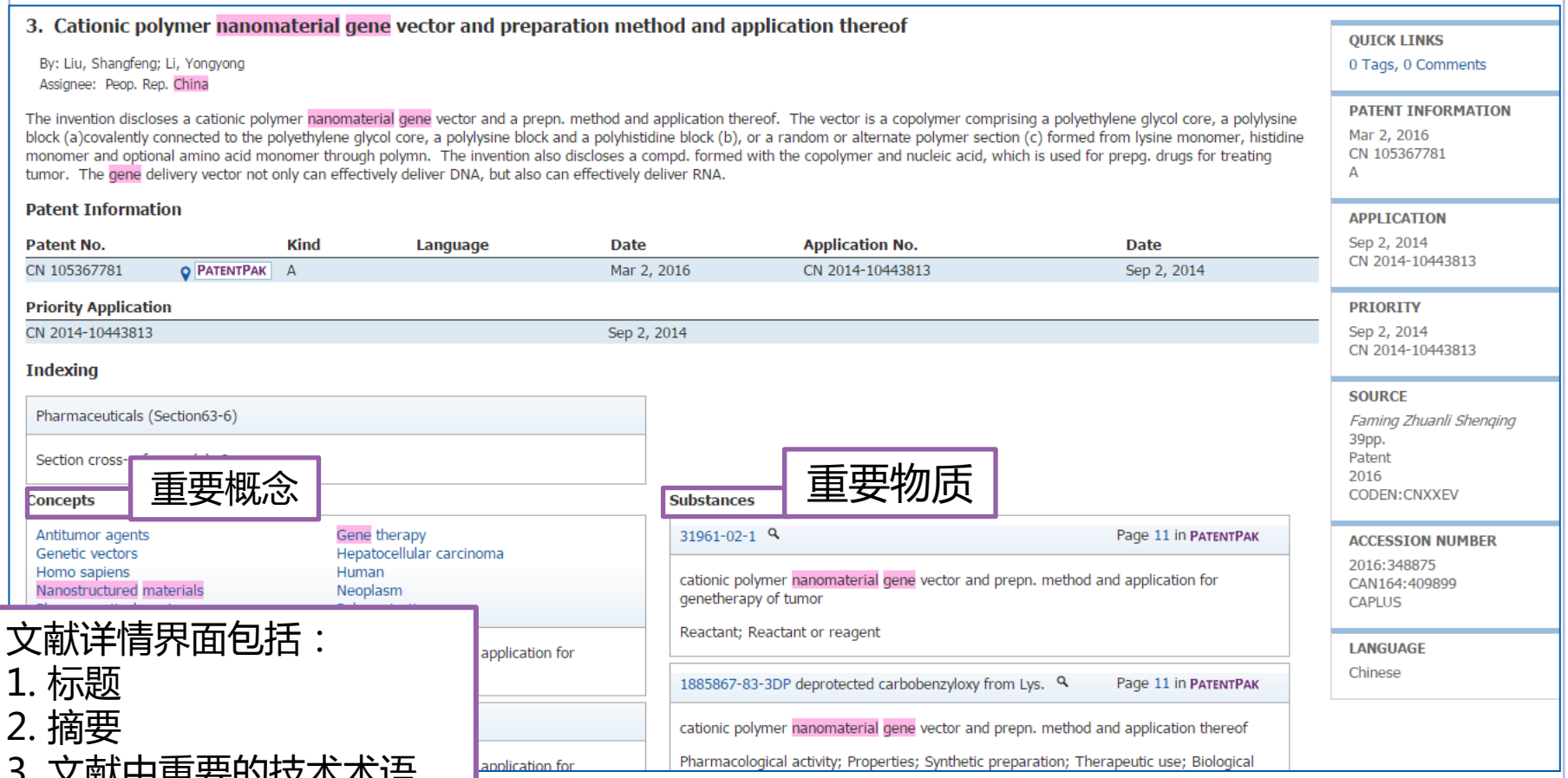
Print：打印成PDF格式

Citation manager: 保存成RIS等格式，可导入EndNote 等文献管理工具

Offline Review：保存成PDF，RTF等格式，用于脱机浏览

SciFinder® A CAS SOLUTION

文献信息—题录、摘要、索引



3. Cationic polymer nanomaterial gene vector and preparation method and application thereof

By: Liu, Shangfeng; Li, Yongyong
Assignee: Peop. Rep. China

The invention discloses a cationic polymer nanomaterial gene vector and a prepn. method and application thereof. The vector is a copolymer comprising a polyethylene glycol core, a polylysine block (a)covalently connected to the polyethylene glycol core, a polylysine block and a polyhistidine block (b), or a random or alternate polymer section (c) formed from lysine monomer, histidine monomer and optional amino acid monomer through polymn. The invention also discloses a compd. formed with the copolymer and nucleic acid, which is used for prepg. drugs for treating tumor. The gene delivery vector not only can effectively deliver DNA, but also can effectively deliver RNA.

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 105367781 PATENTPAK	A		Mar 2, 2016	CN 2014-10443813	Sep 2, 2014

Priority Application

CN 2014-10443813	Sep 2, 2014

Indexing

Pharmaceuticals (Section63-6)

Section cross-

重要概念

Concepts

Antitumor agents
Genetic vectors
Homo sapiens
Nanostructured materials
Gene therapy
Hepatocellular carcinoma
Human
Neoplasm

application for

application for

重要物质

Substances

31961-02-1 Page 11 in PATENTPAK

cationic polymer nanomaterial gene vector and prepn. method and application for genetherapy of tumor

Reactant; Reactant or reagent

1885867-83-3DP deprotected carbobenzyloxy from Lys. Page 11 in PATENTPAK

cationic polymer nanomaterial gene vector and prepn. method and application thereof

Pharmacological activity; Properties; Synthetic preparation; Therapeutic use; Biological

QUICK LINKS
0 Tags, 0 Comments

PATENT INFORMATION
Mar 2, 2016
CN 105367781
A

APPLICATION
Sep 2, 2014
CN 2014-10443813

PRIORITY
Sep 2, 2014
CN 2014-10443813

SOURCE
Faming Zhuanli Shenqing
39pp.
Patent
2016
CODEN:CNXXEV

ACCESSION NUMBER
2016:348875
CAN164:409899
CAPLUS

LANGUAGE
Chinese

文献详情界面包括：
1. 标题
2. 摘要
3. 文献中重要的技术术语
4. 文献中重要的物质
5. 书目信息
6. 获得文献中的物质，反应
7. 参考文献
8. 链接原文

SCIFINDER® A CAS SOLUTION

文献检索小结

- 主题检索时，使用介词 in, with, of 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
- 尝试将不同的Analyze/Refine功能组合起来用，会有更多的收益
- 使用Categorize可以让系统来实现自动分类

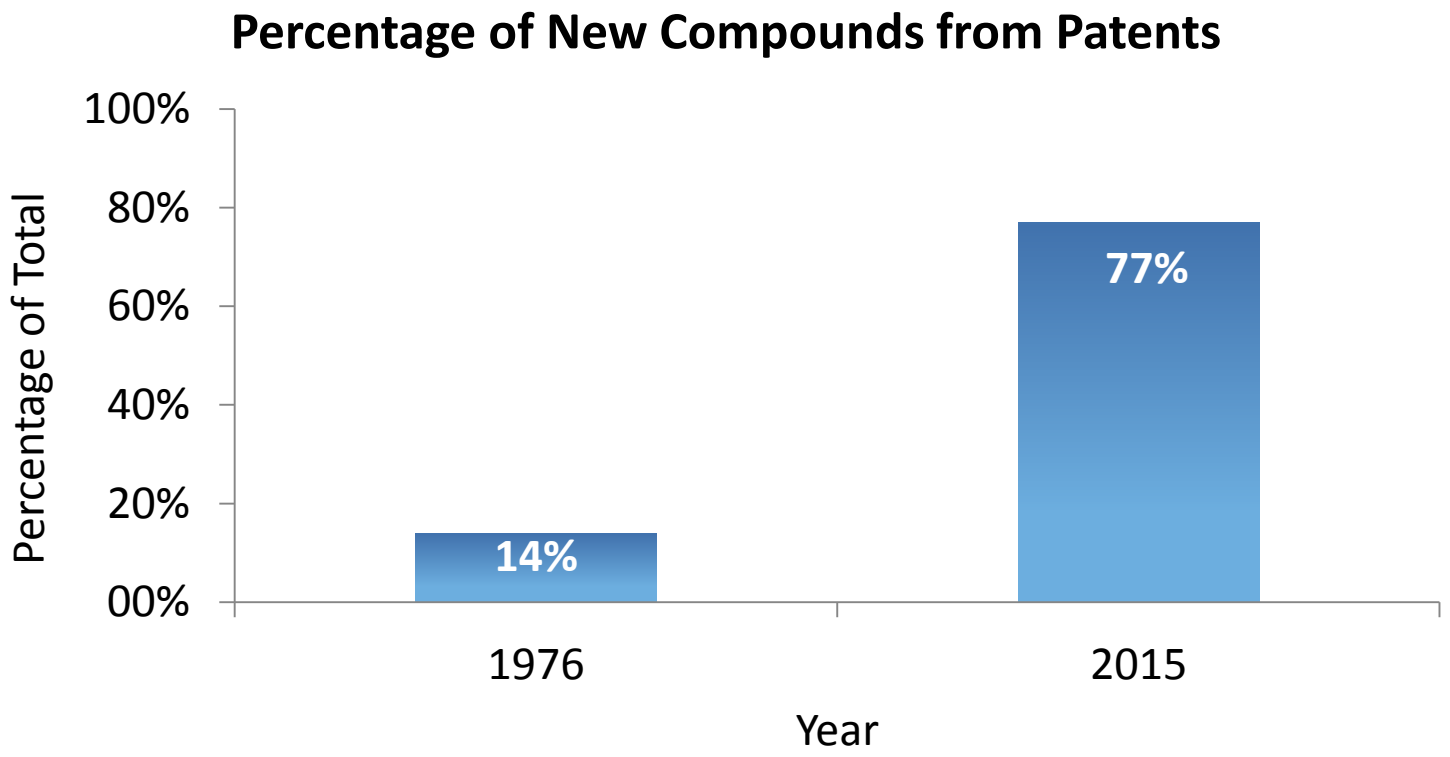
SCIFINDER® A CAS SOLUTION

PatentPak™

专利工作流程解决方案

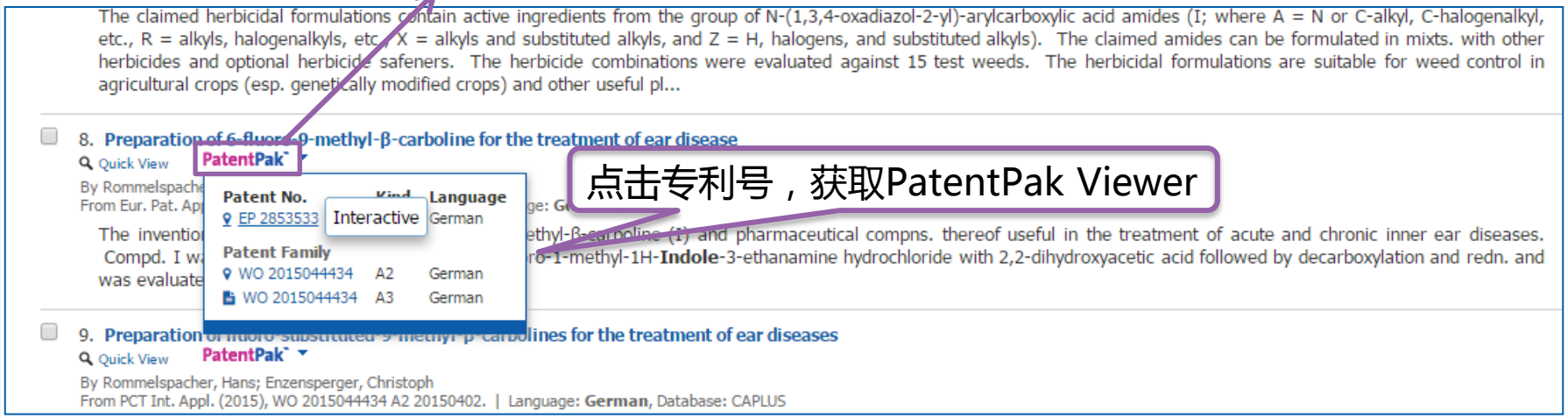
SciFinder® A CAS SOLUTION

越来越多的新化合物倾向于首先通过专利公布

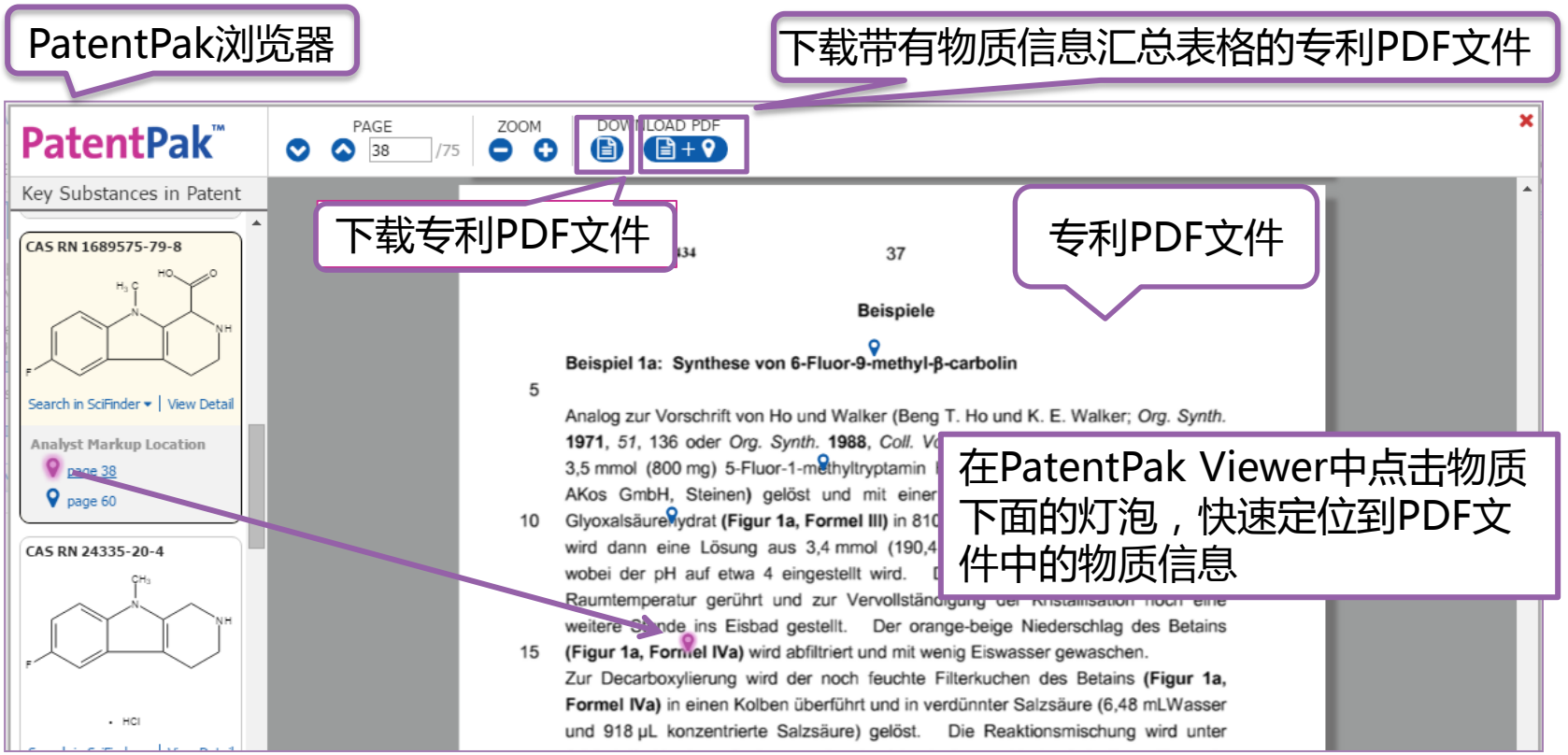


PatentPak——专利工作流程解决方案

在SciFinder检索结果中，看到PatentPak图标即可点击



PatentPak——专利工作流程解决方案



SciFinder® A CAS SOLUTION

节省您最宝贵的资源——时间

- 即时获得来自世界上31家专利授权机构的逾900万份专利PDF文件，且数量持续增加
- 专利族涵盖了多种语言
- 通过CAS登记号获得物质在专利文献中的相关信息
- 专利研究安全保密
- 每日更新
- SciFinder检索功能中内置交互式浏览器

SCIFINDER® A CAS SOLUTION

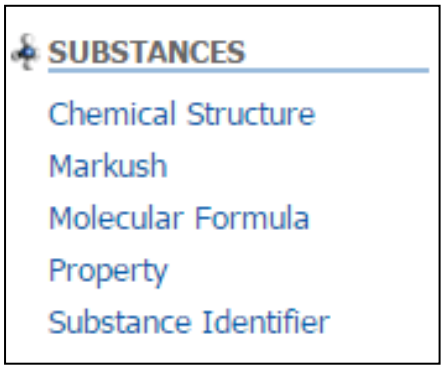
提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak）
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

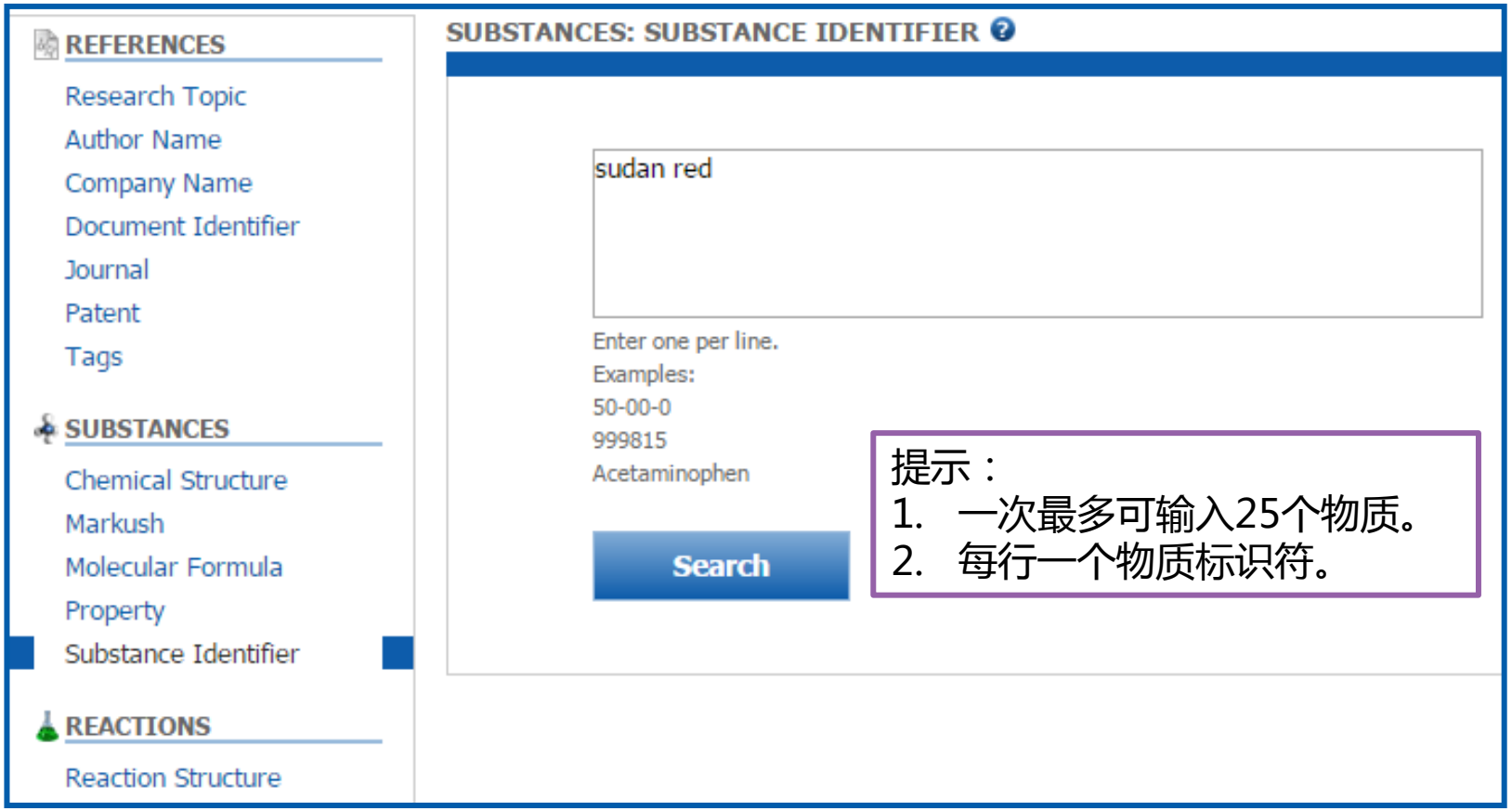
SciFinder检索选项——物质检索

- 物质检索方法
  - —结构式检索
  - —分子式检索
  - —理化性质检索
  - —物质标识符检索：化学名称，CAS RN



- 物质检索策略推荐
  - —有机化合物，天然产物：结构检索
  - —无机物，合金：分子式检索
  - —高分子化合物：分子式检索和结构检索

物质检索——标识符检索

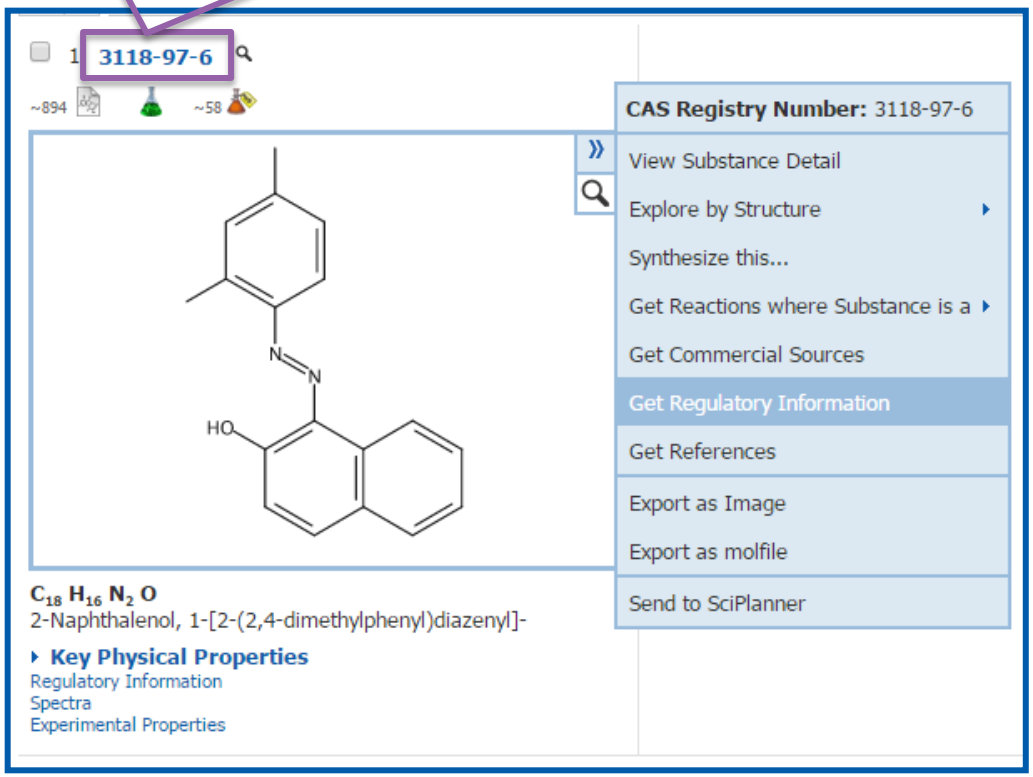


物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

SciFinder® A CAS SOLUTION

SciFinder中的物质记录

点击CAS RN 获得物质详细信息



在SciFinder中，鼠标滑过物质，即可打开物质标准菜单，获得与物质相关的所有内容

SciFinder中的物质记录

SUBSTANCE DETAIL

Get References | Get Reactions | Get Commercial Sources

Return

由物质获得文献，反应，供应商等信息

CAS Registry Number 3118-97-6

~894 ~58

$C_{18}H_{16}N_2O$

2-Naphthalenol, 1-[2-(2,4-dimethylphenyl)diazenyl]-

Molecular Weight
276.33

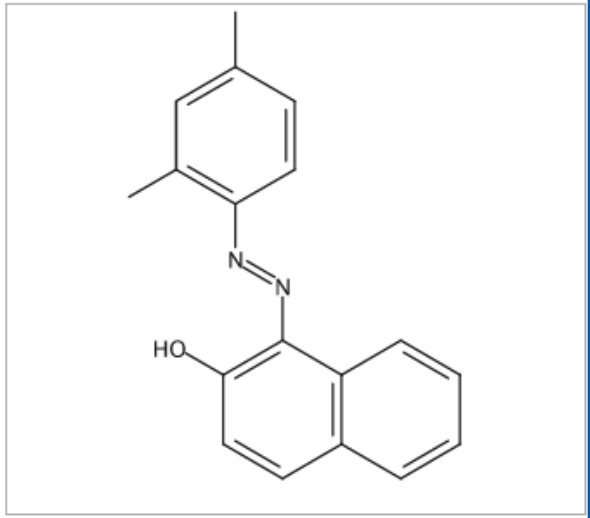
Melting Point (Experimental)
Value: 166 °C

Boiling Point (Predicted)
Value: 476.7±40.0 °C | Condition: Press: 760 Torr

Density (Predicted)
Value: 1.14±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)
Value: 13.52±0.50 | Condition: Most Acidic Temp: 25 °C

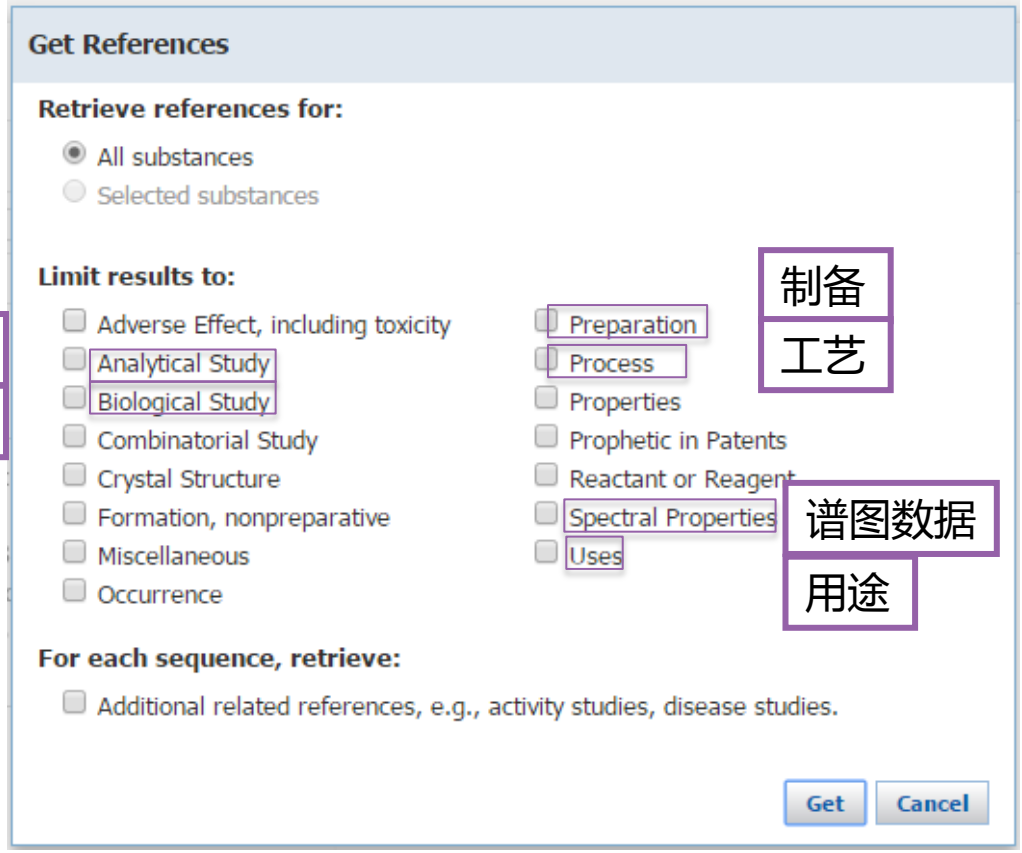
Other Names
2-Naphthalenol, 1-[(2,4-dimethylphenyl)azo]- (9CI)
C.I. Solvent Orange 7 (7CI,8CI)
Sudan Red (6CI)
1-[2-(2,4-Dimethylphenyl)diazenyl]-2-naphthalenol
AF Red No. 5
View more...



物质详情

SciFinder® A CAS SOLUTION

通过物质获得文献



分析化学

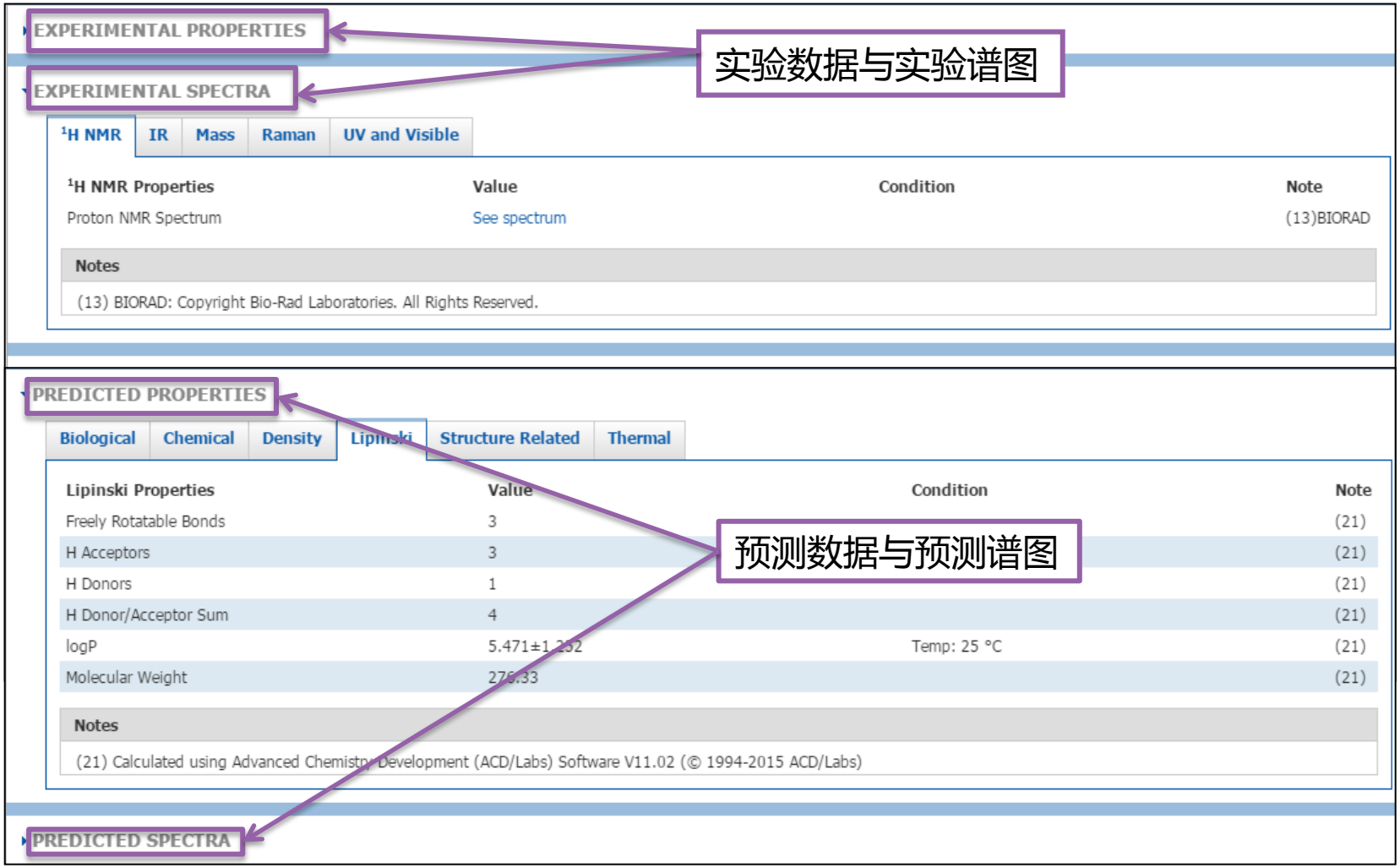
生物研究

制备

工艺

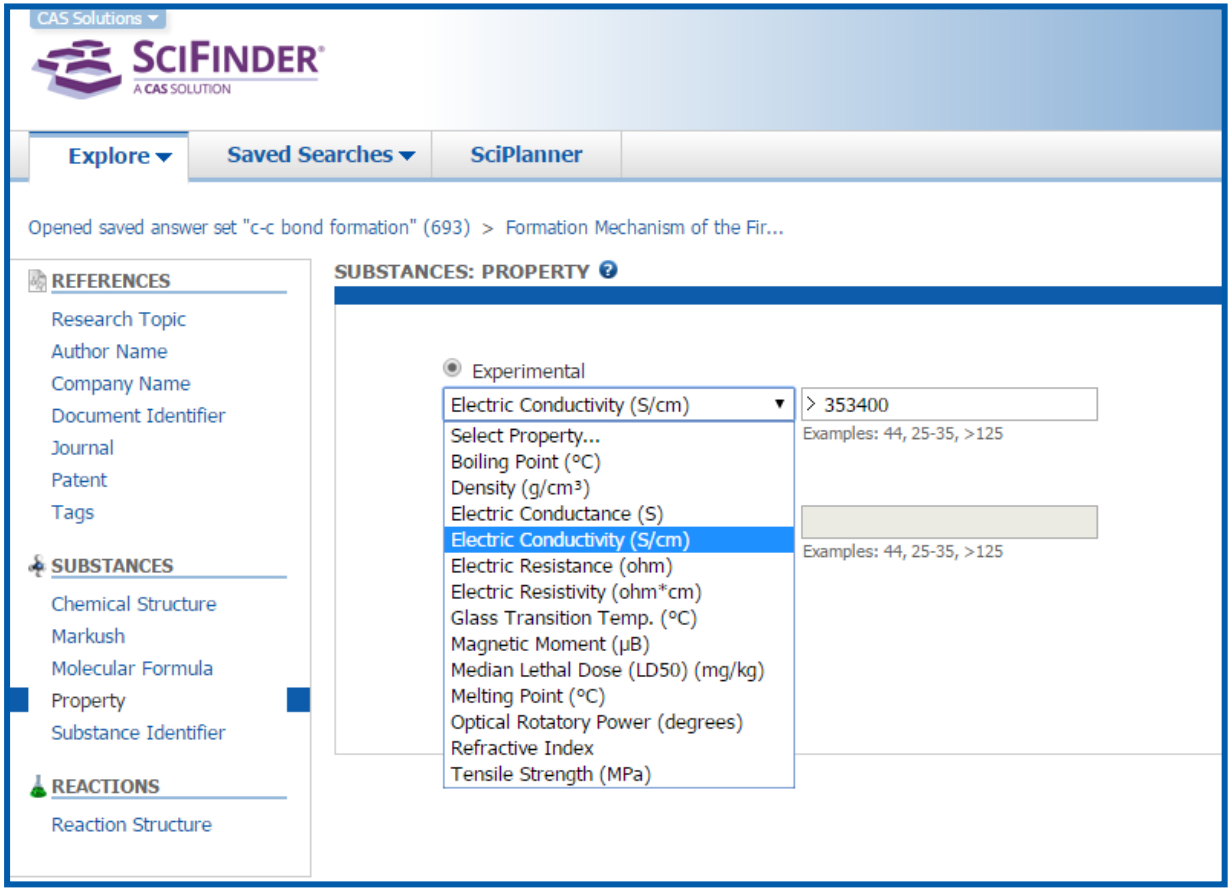
谱图数据

用途



SciFinder® A CAS SOLUTION

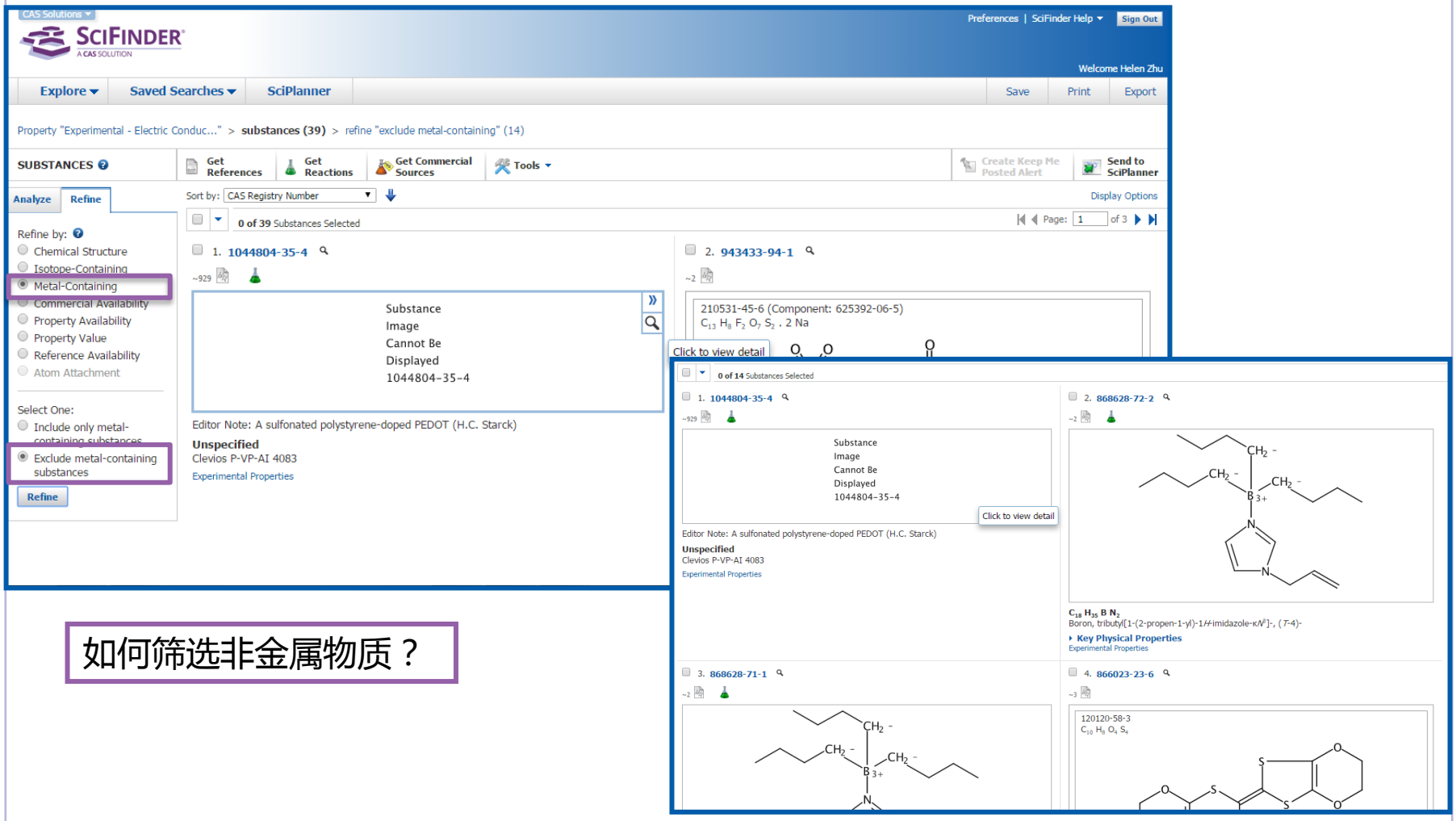
物质检索——Property explore



寻找导电率比铜的60%大的非金属材料

SciFinder
A CAS SOLUTION

物质结果集的筛选——Refine



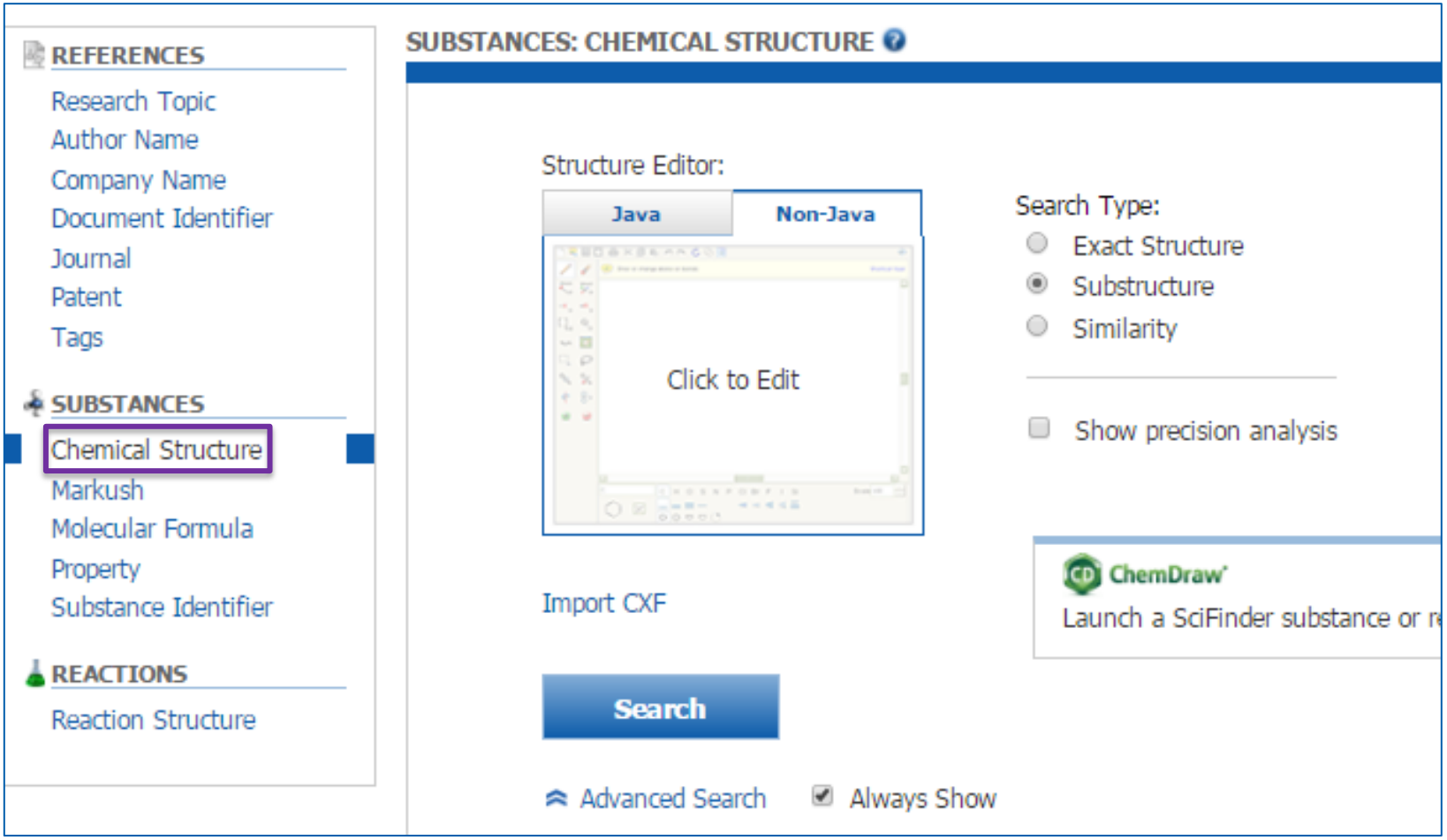
如何筛选非金属物质？

物质检索——分子式

分子式输入需要遵守Hill排序规则：不含碳化合物，按元素符号的字母顺序排列；分子式为含碳化合物时，则“C”在前；如有氢则紧随其后，其它元素符号按字母顺序排在氢的后面

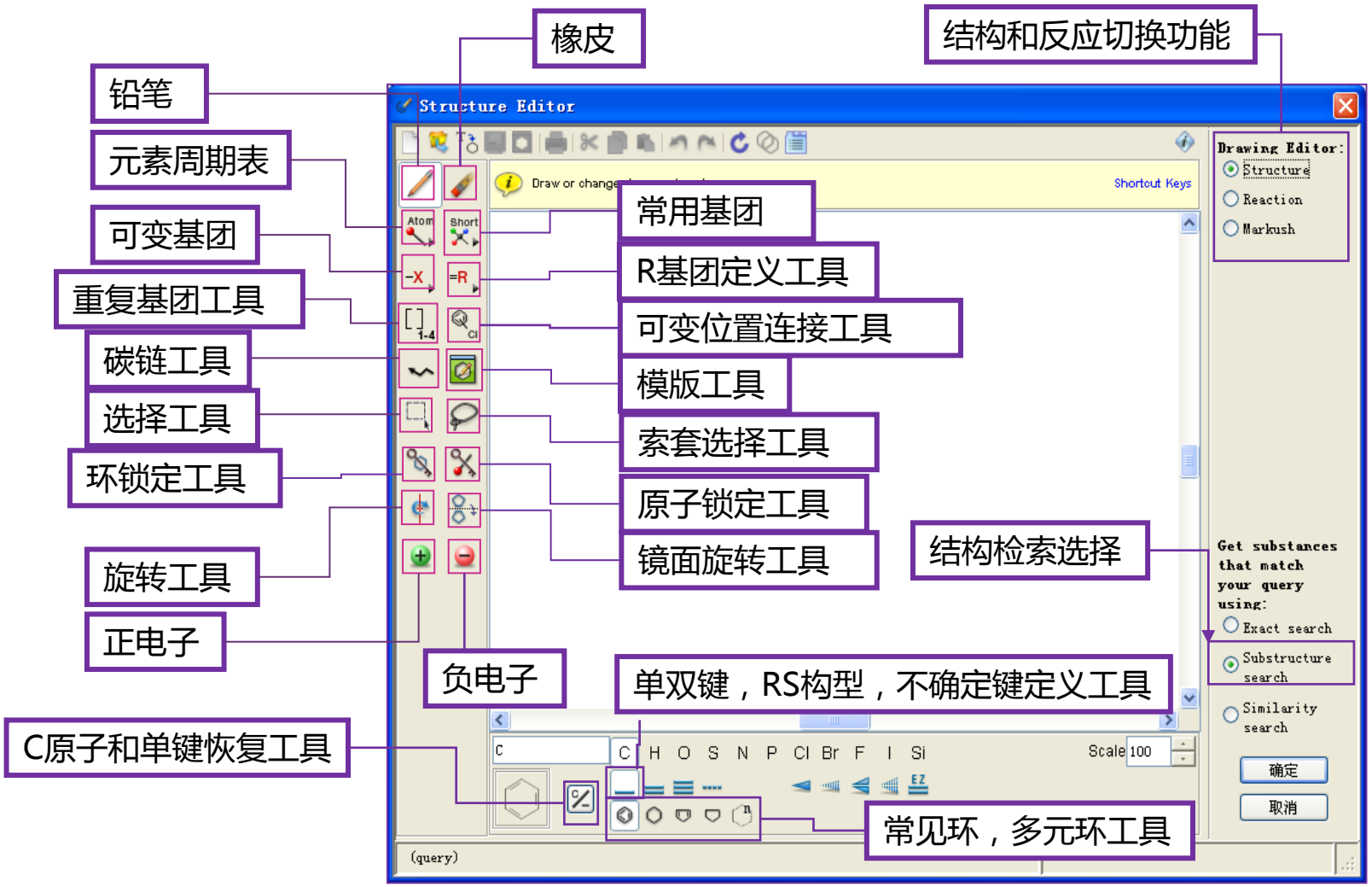
SciFinder® A CAS SOLUTION

物质检索——结构

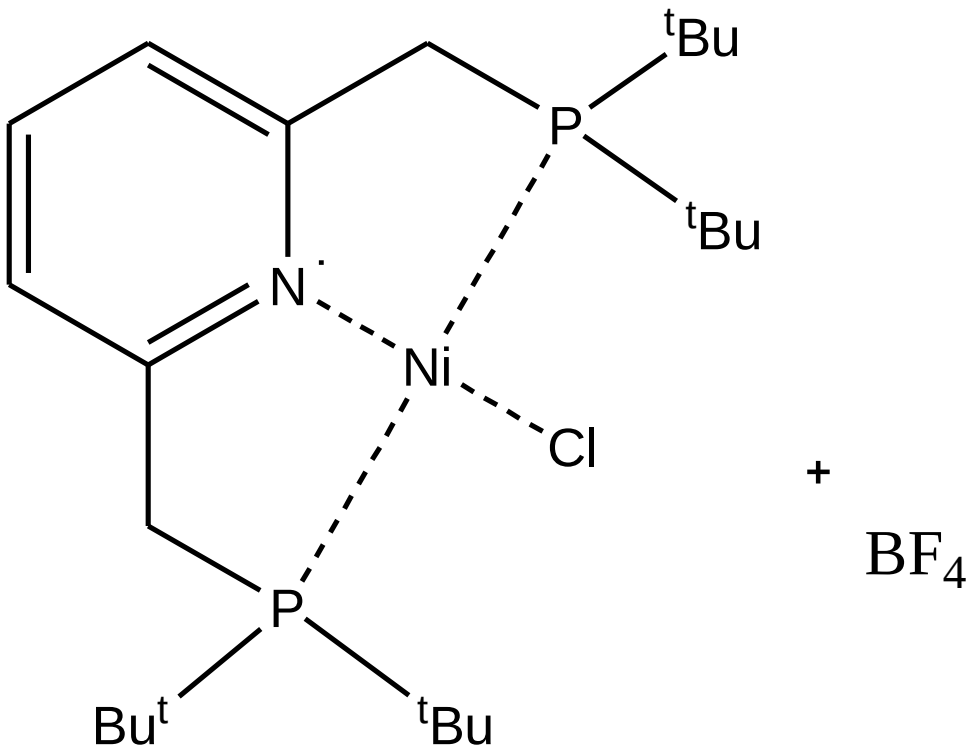


SciFinder® A CAS SOLUTION

物质检索——结构


铅笔
橡皮
结构和反应切换功能
元素周期表
可变基团
重复基团工具
碳链工具
选择工具
环锁定工具
旋转工具
正电子
C原子和单键恢复工具
负电子
常用基团
R基团定义工具
可变位置连接工具
模版工具
索套选择工具
原子锁定工具
镜面旋转工具
结构检索选择
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
Scale 100
(query)

物质检索——精确结构检索

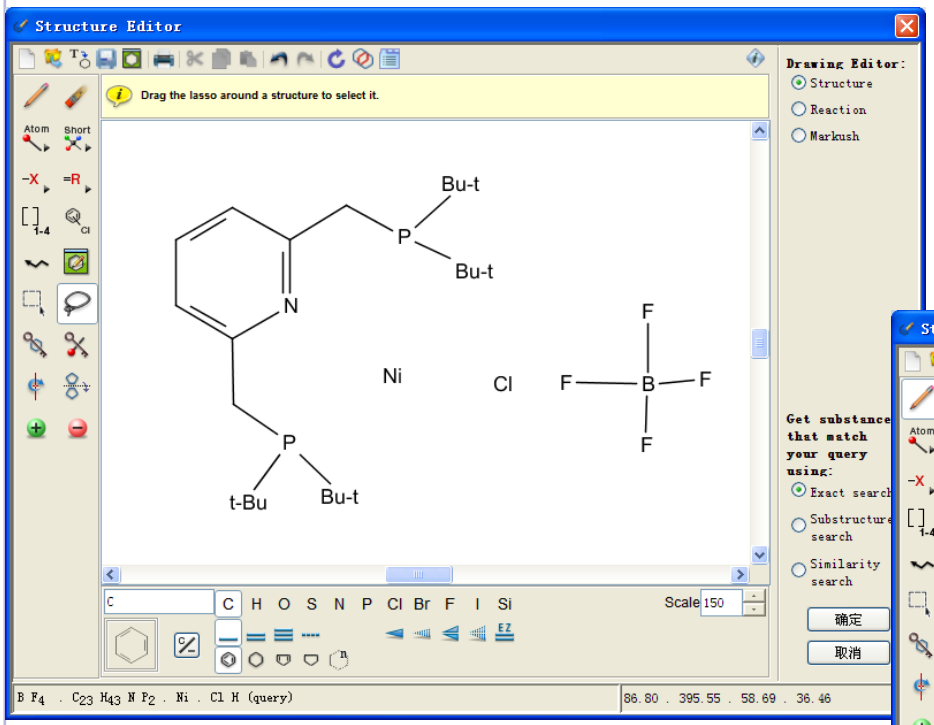


+ BF_4

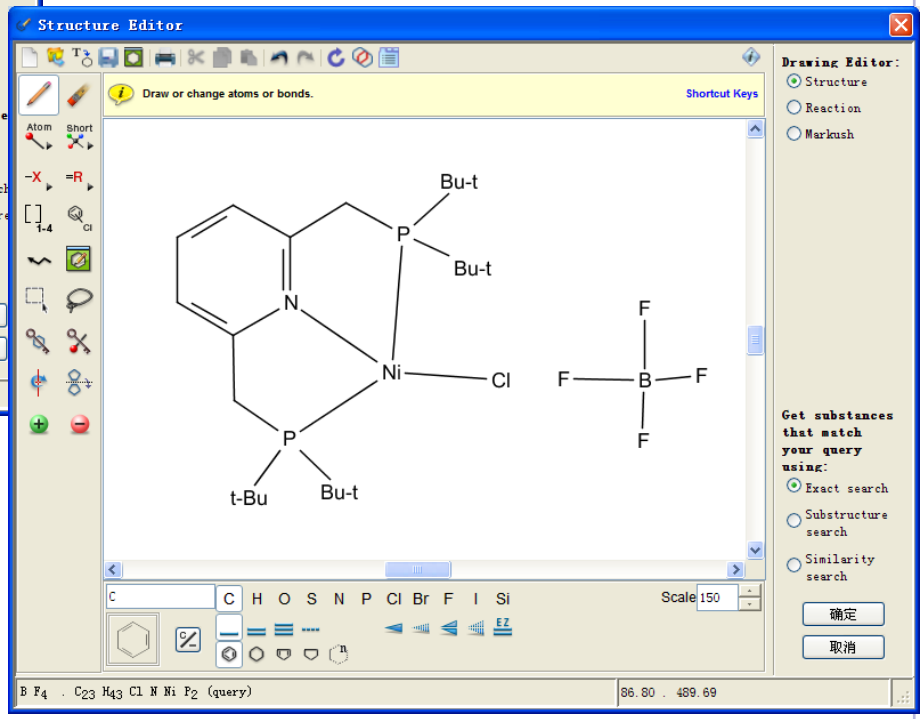
该结构中包含：

配体
金属
阳离子
阴离子

物质检索——精确结构检索



任何一种结构,使用精确结构都可以检索到

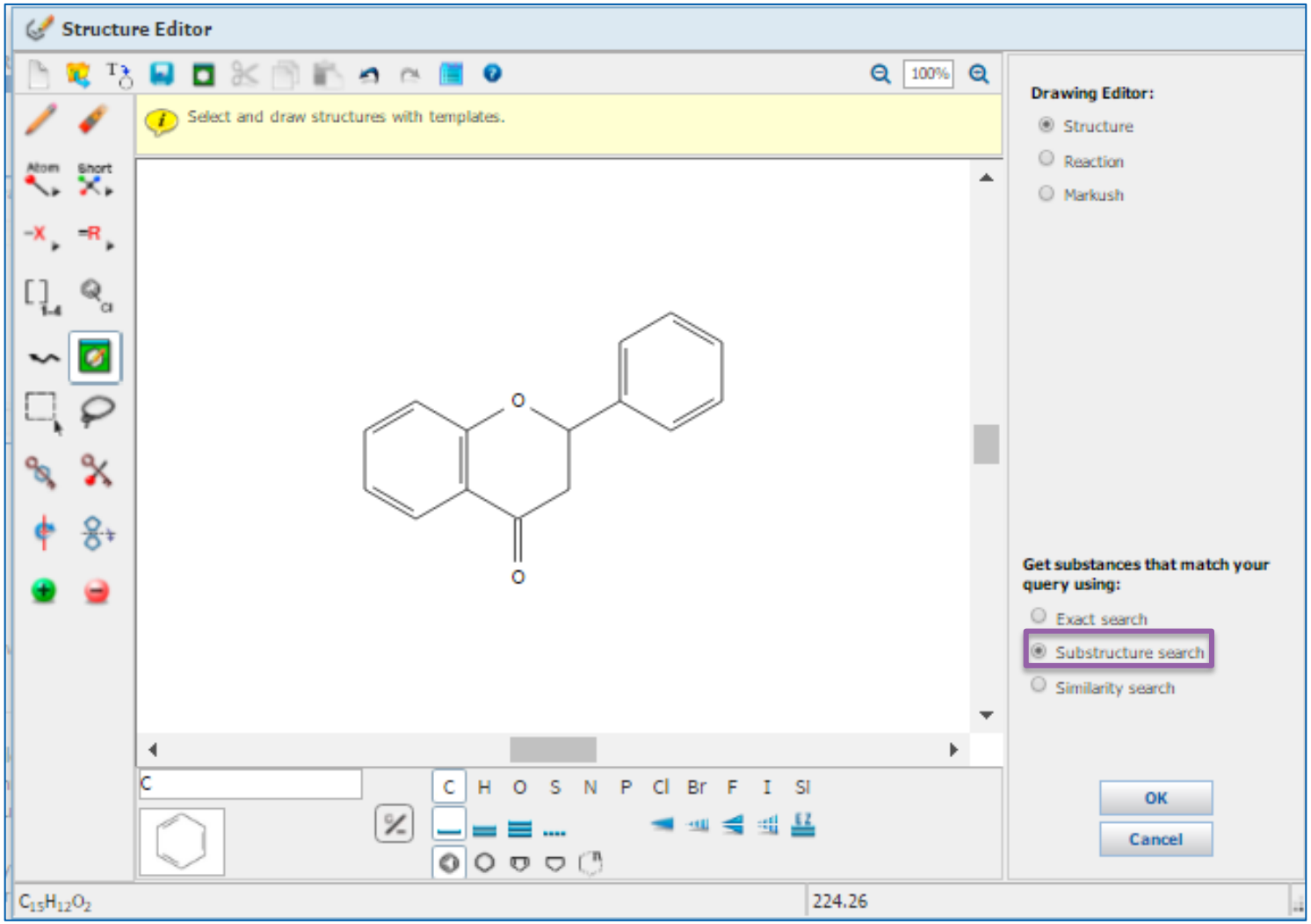


物质检索——精确结构检索

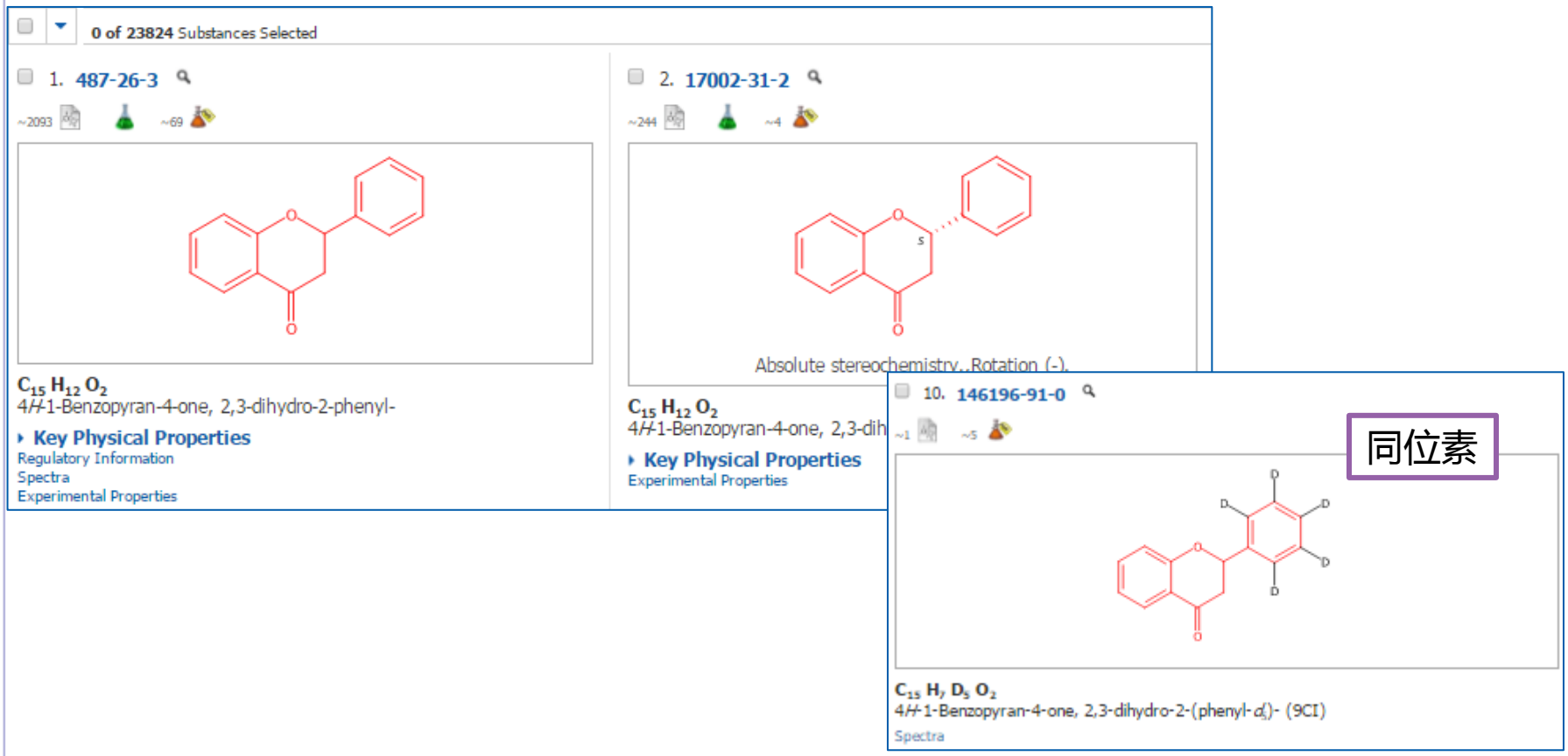
- 精确结构检索：

获得被检索结构的盐，混合物，配合物，聚合物等，被检结构不能被取代

物质检索——亚结构检索


Structure Editor
100%
Select and draw structures with templates.
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search
OK
Cancel
C H O S N P Cl Br F I Si
$C_{15}H_{12}O_2$
224.26

物质检索——亚结构检索

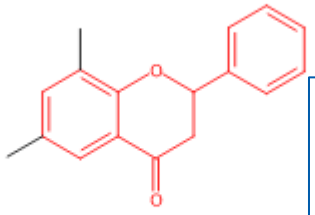


SciFinder® A CAS SOLUTION

亚结构检索结果

281. 123251-10-5

取代物



$C_{17}H_{16}O_2$

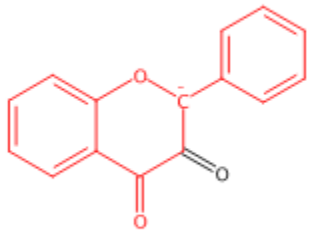
4*H*-1-Benzopyran-4-one, 2,3-dihydro-6,8-dimethyl

Key Physical Properties

Experimental Properties

295. 780723-19-5

离子

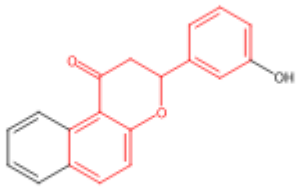


$C_{15}H_9O_3$

2*H*-1-Benzopyran-3,4-dione, 2-phenyl-, ion(1-)

284. 136116-23-9

稠环物质



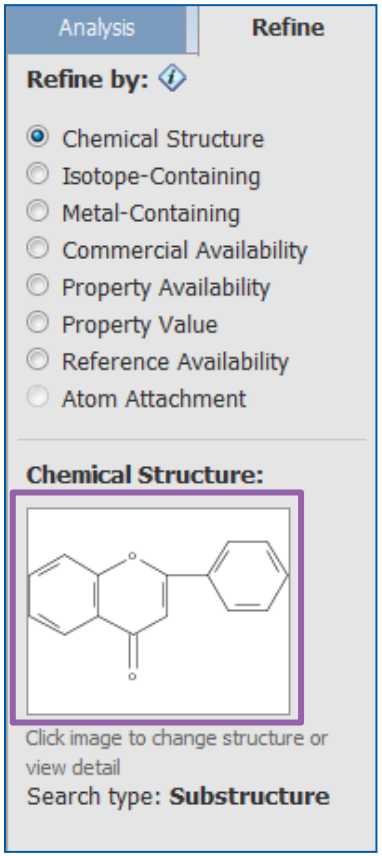
$C_{19}H_{14}O_3$

1*H*-Naphtho[2,1-*b*]pyran-1-one, 2,3-dihydro-3-(3-hydroxyphenyl)-

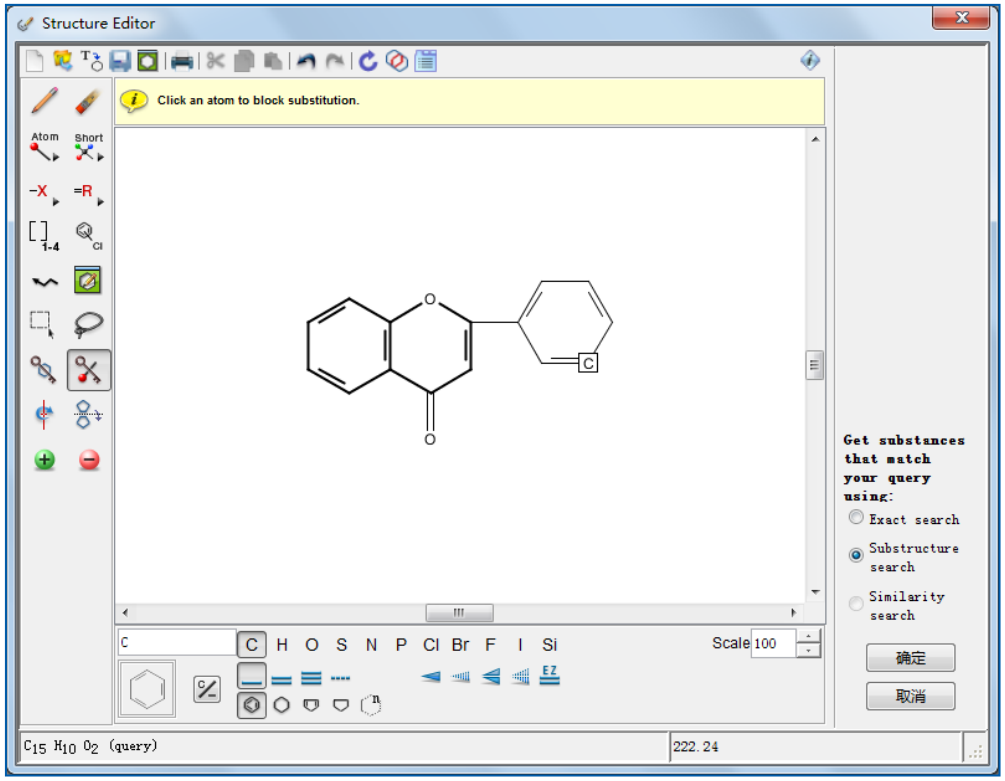
Key Physical Properties

SciFinder® A CAS SOLUTION

亚结构检索结果的限定



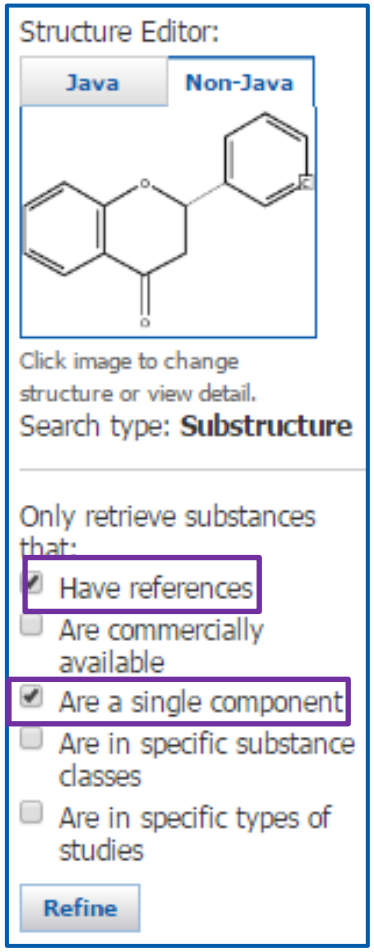
化学结构的再次限定

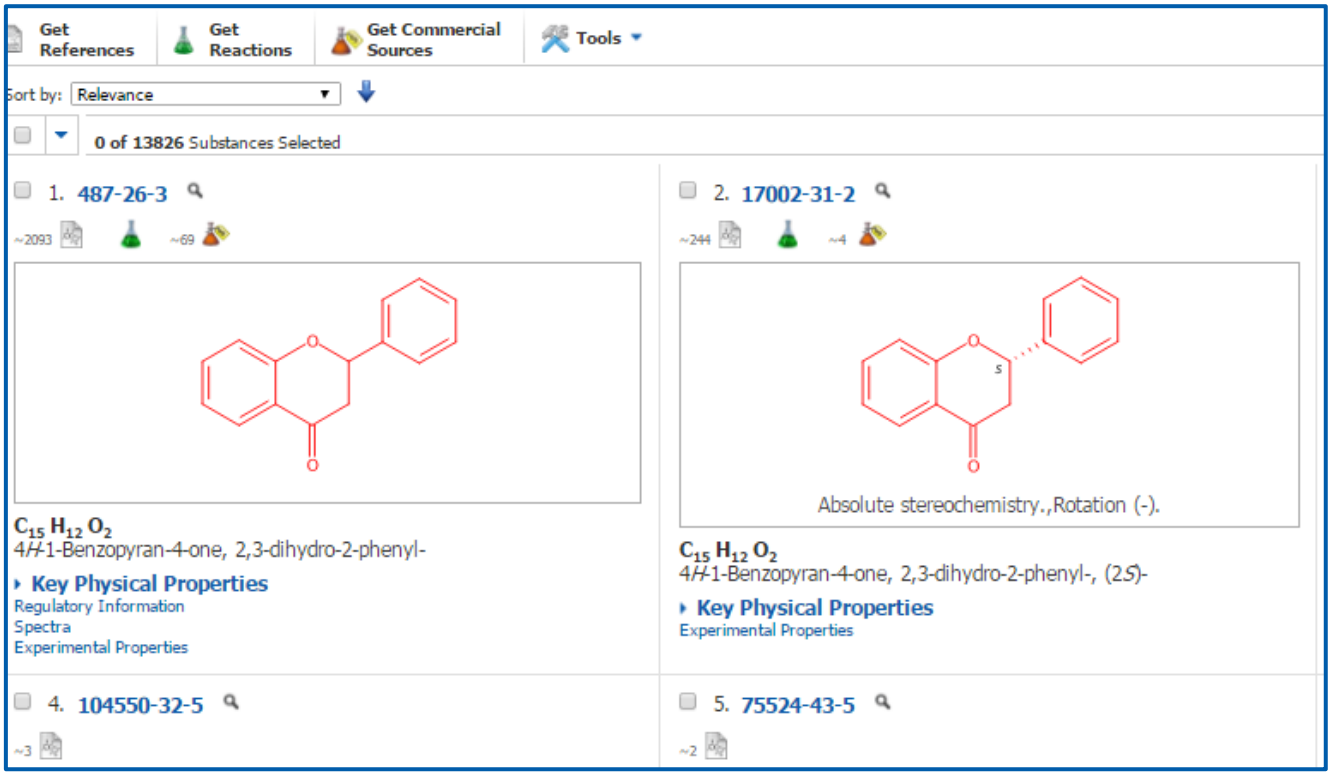


环锁定

原子锁定

亚结构检索结果的限定


Structure Editor:
Java
Non-Java
Click image to change structure or view detail.
Search type: Substructure
Only retrieve substances that:
Have references
Are commercially available
Are a single component
Are in specific substance classes
Are in specific types of studies
Refine

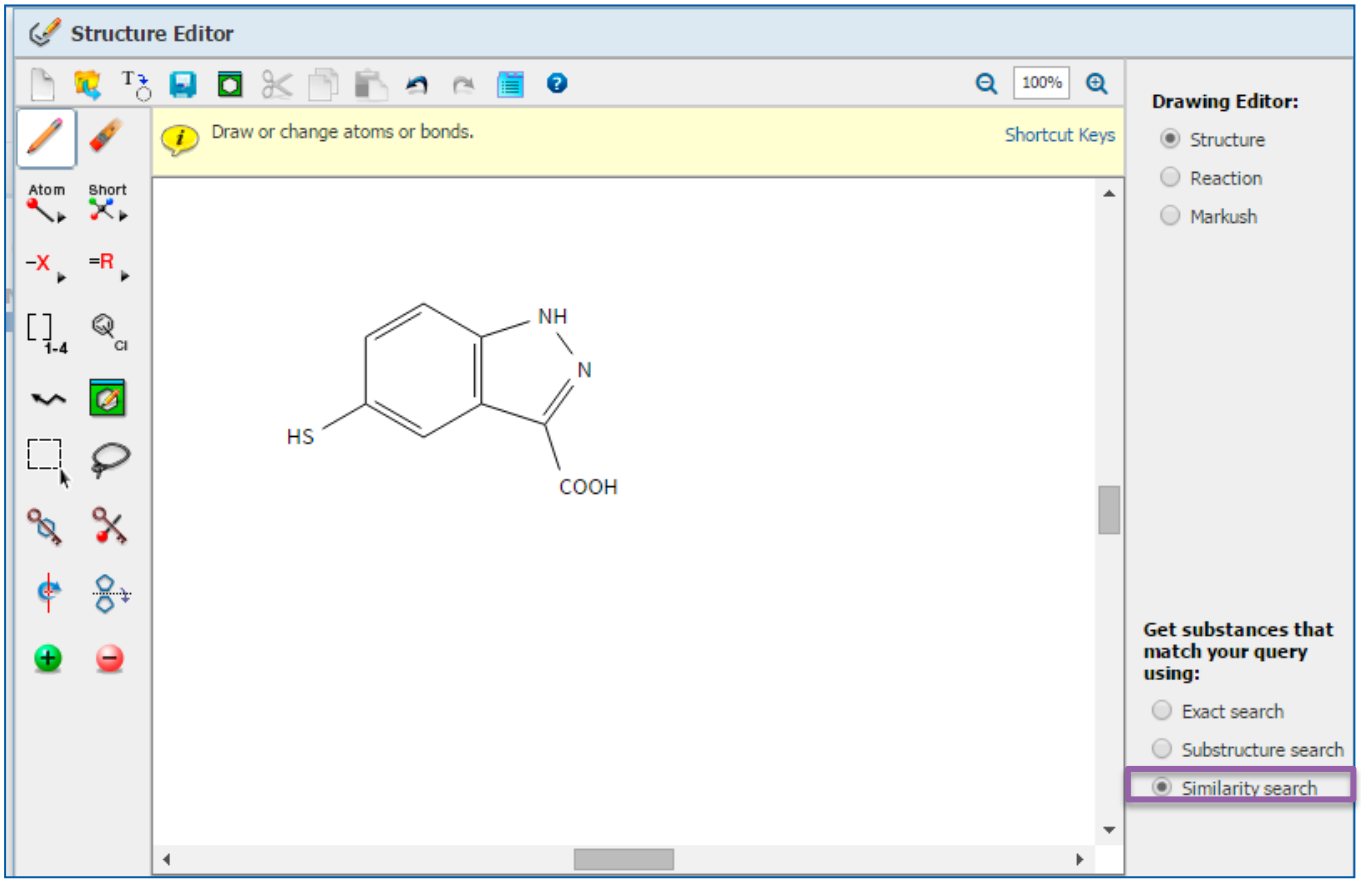

Get References
Get Reactions
Get Commercial Sources
Tools
Sort by: Relevance
0 of 13826 Substances Selected
1. 487-26-3
2. 17002-31-2
Absolute stereochemistry.,Rotation (-).
C15 H12 O2
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Key Physical Properties
Regulatory Information
Spectra
Experimental Properties
C15 H12 O2
4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-, (2S)-
Key Physical Properties
Experimental Properties
4. 104550-32-5
5. 75524-43-5

物质检索——亚结构检索

- 亚结构检索：

包括精确结构检索结果，及被检索结构的修饰结构

物质检索——相似结构检索


Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Atom
Short
NH
N
HS
COOH
Drawing Editor:
Structure
Reaction
Markush
Get substances that match your query using:
Exact search
Substructure search
Similarity search

相似结构检索结果

Select All Deselect All

0 of 6 Similarity Candidates Selected	Substances
≥ 99 (most similar)	0
95-98	0
90-94	0
85-89	11
80-84	34
75-79	84
70-74	267
65-69	696
0-64 (least similar)	1818

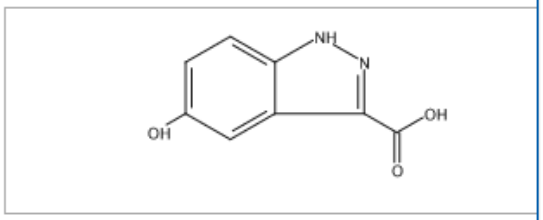
Get Substances

评分越高，相似度越高，结构越相似

Score: 88

1. **885518-94-5**

~1 ~35



取代基变化

$C_8H_6N_2O_3$

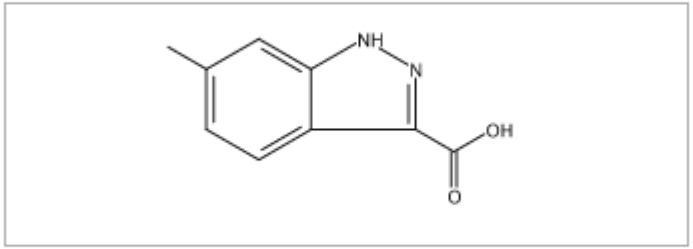
1*H*-Indazole-3-carboxylic acid, 5-hydroxy-

Key Physical Properties

Score: 86

5. **858227-12-0**

~7 ~41



取代基位置变化

$C_9H_8N_2O_2$

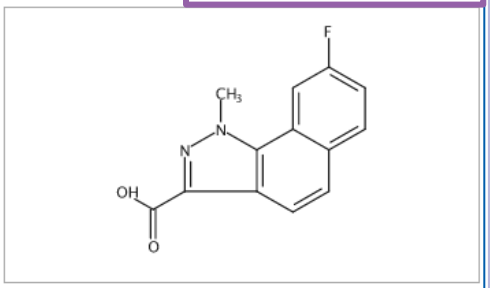
1*H*-Indazole-3-carboxylic acid, 6-methyl-

Key Physical Properties

Score: 65

541. **1100422-**

~1



母体结构变化

$C_{13}H_9FN_2O_2$

1*H*-Benz[*g*]indazole-3-carboxylic acid, 8-fluoro-1-methyl-

Key Physical Properties

SciFinder® A CAS SOLUTION

物质检索——相似结构检索

- 相似结构检索：

获得片段或整体结构与被检索结构相似的结果，母体结构可以被取代，也可以被改变

提纲

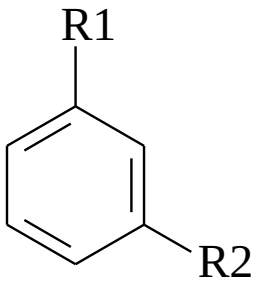
- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索（PatentPak)
  - 物质检索
  - Markush检索
  - 反应检索 （ MethodsNow Synthesis ）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SCIFINDER® A CAS SOLUTION

Markush检索

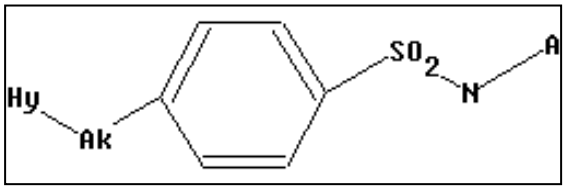
- 具体物质[Specific Substance]：
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 预测性物质[Prophetic Substance]：
  — 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质
  — 专利中所陈述的预测物质，不会被分配CAS RN
  — Markush检索，能检索到通过结构检索检不到的专利

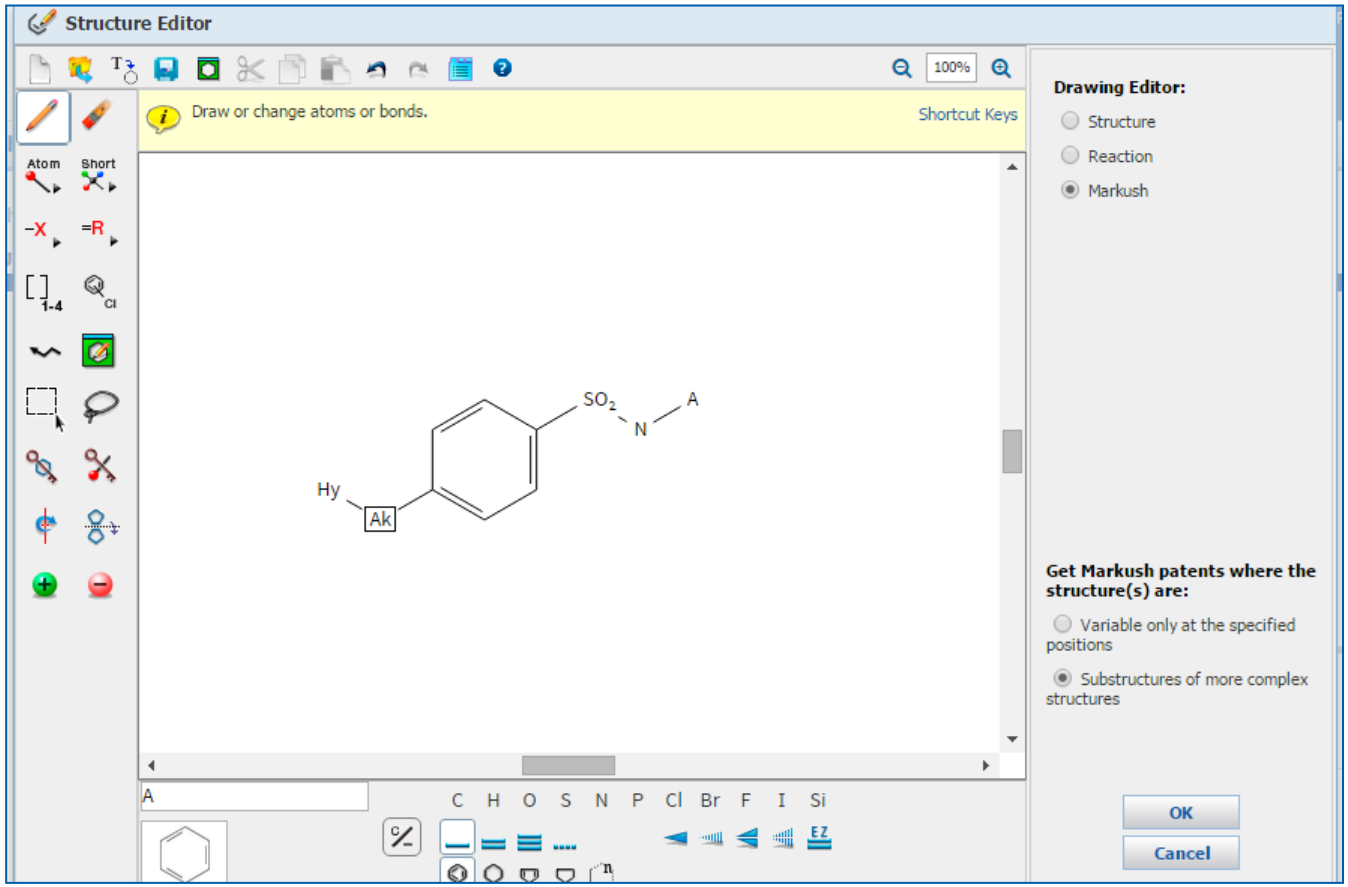


R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH_2–halogen, —CH(–halogen)–CH_3,



可用SciFinder中的Markush检索查看专利中化合物结构保护范围。



提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
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  - 反应检索（MethodsNow Synthesis）
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  - MethodsNow
- SciFinder常见问题及解决

SciFinder检索选项——反应检索

- 反应检索方法

  结构式

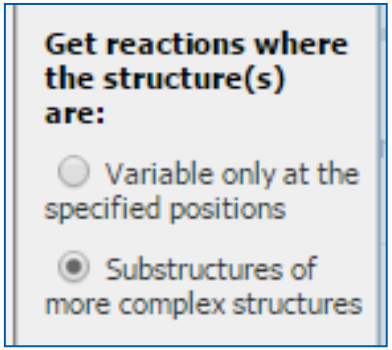
- 常用获取方法

  已知物质：由物质获取反应

  已知文献：从文献中获取反应

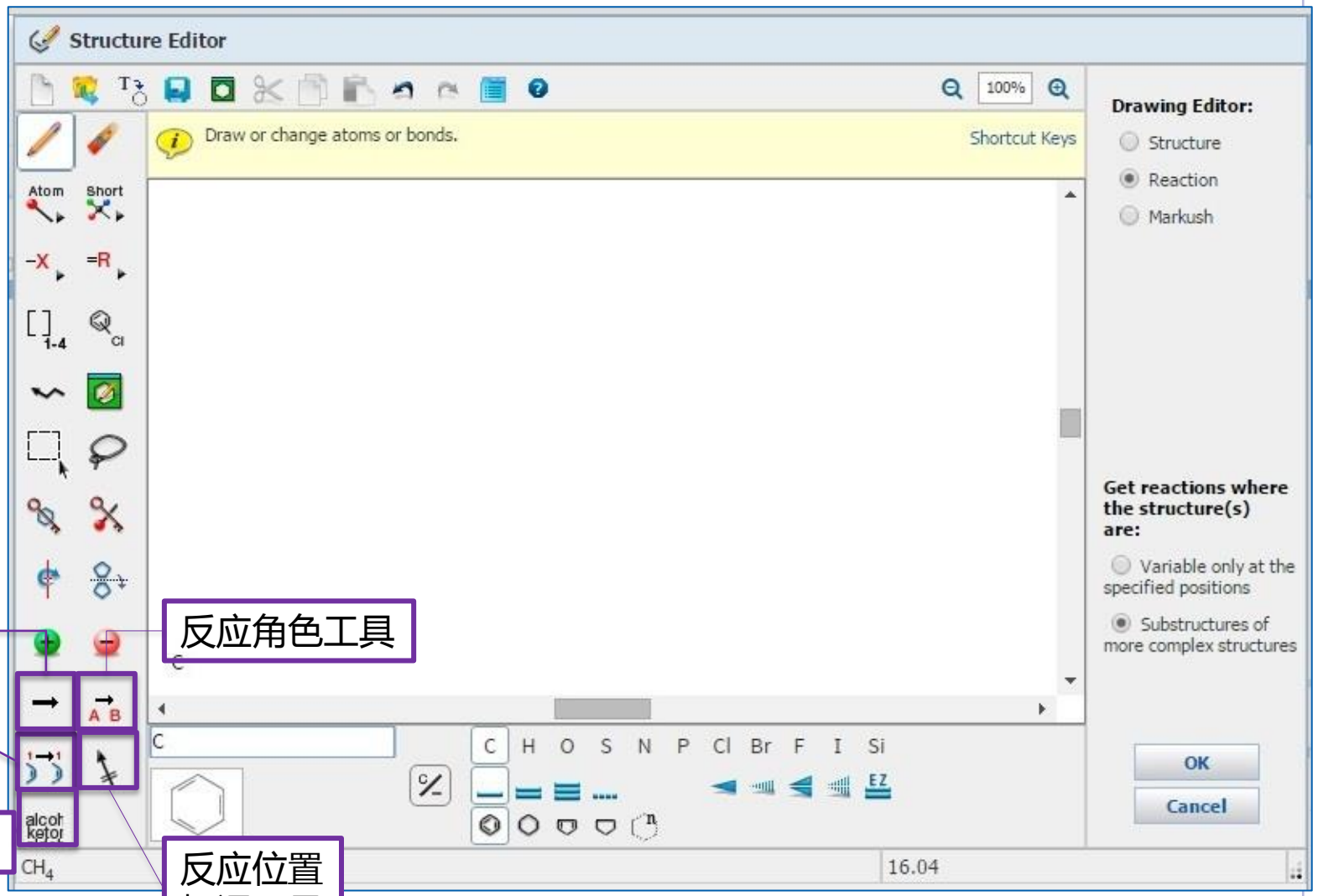
  精确结构反应检索

  亚结构反应检索

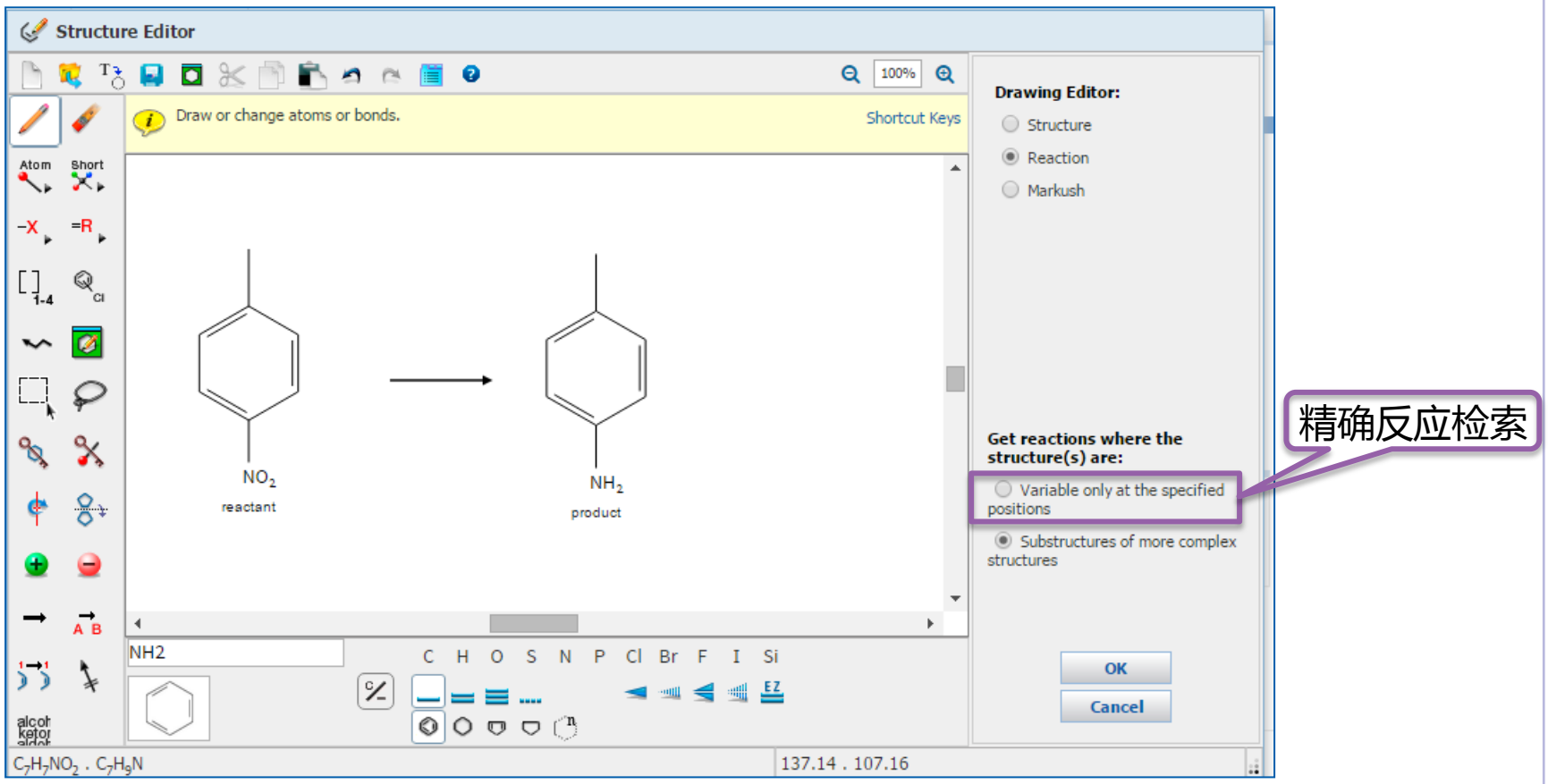


SciFinder® A CAS SOLUTION

反应绘制工具

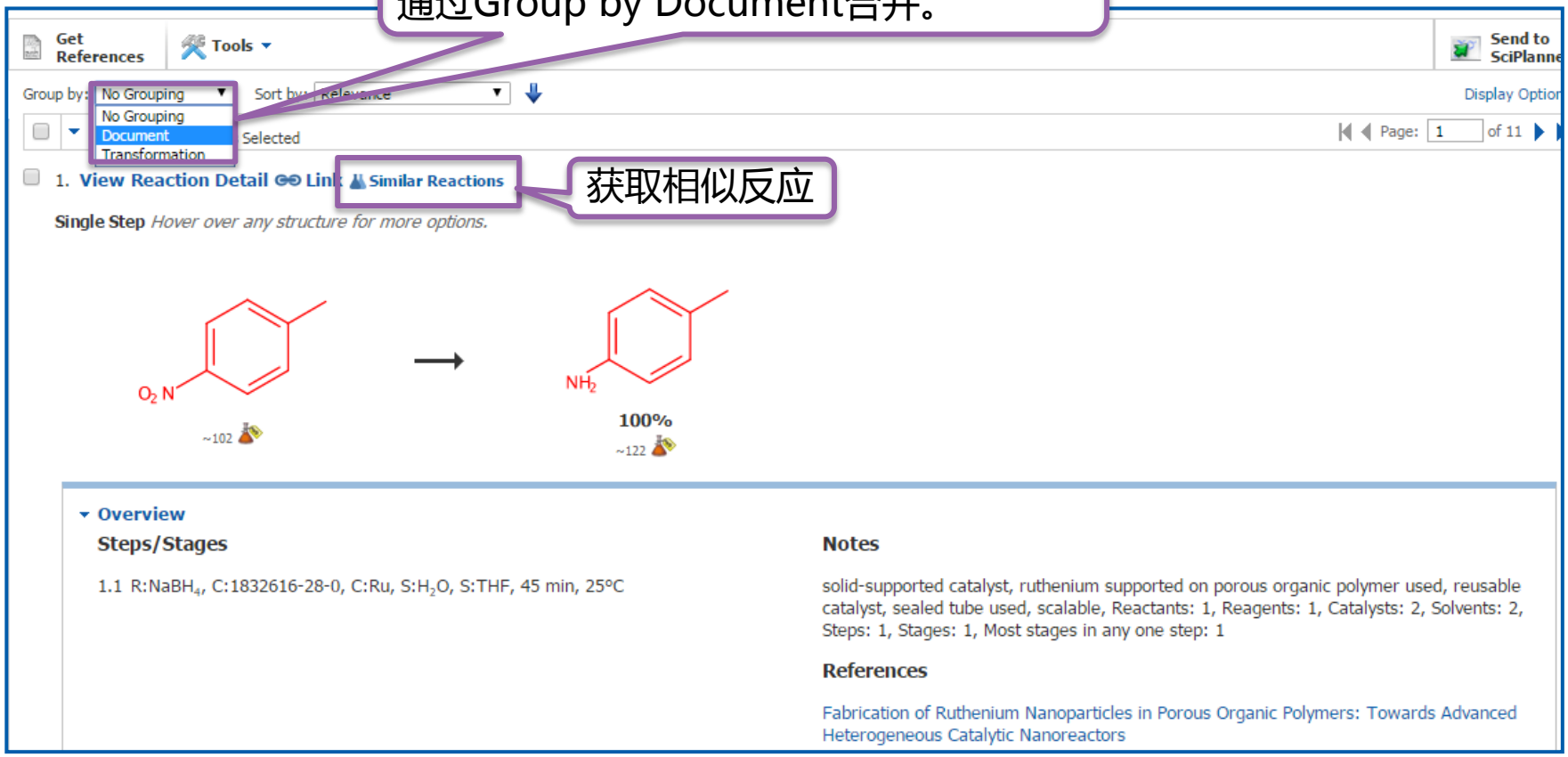

Structure Editor
100%
Draw or change atoms or bonds.
Shortcut Keys
Drawing Editor:
Structure
Reaction
Markush
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
OK
Cancel
C H O S N P Cl Br F I Si
CH4
16.04
反应箭头
反应角色工具
反应原子标记工具
官能团列表
反应位置标记工具

SciFinder反应检索——精确反应检索



反应检索结果

浏览记录，发现很多反应来自同一篇文献，通过Group by Document合并。



SciFinder® A CAS SOLUTION

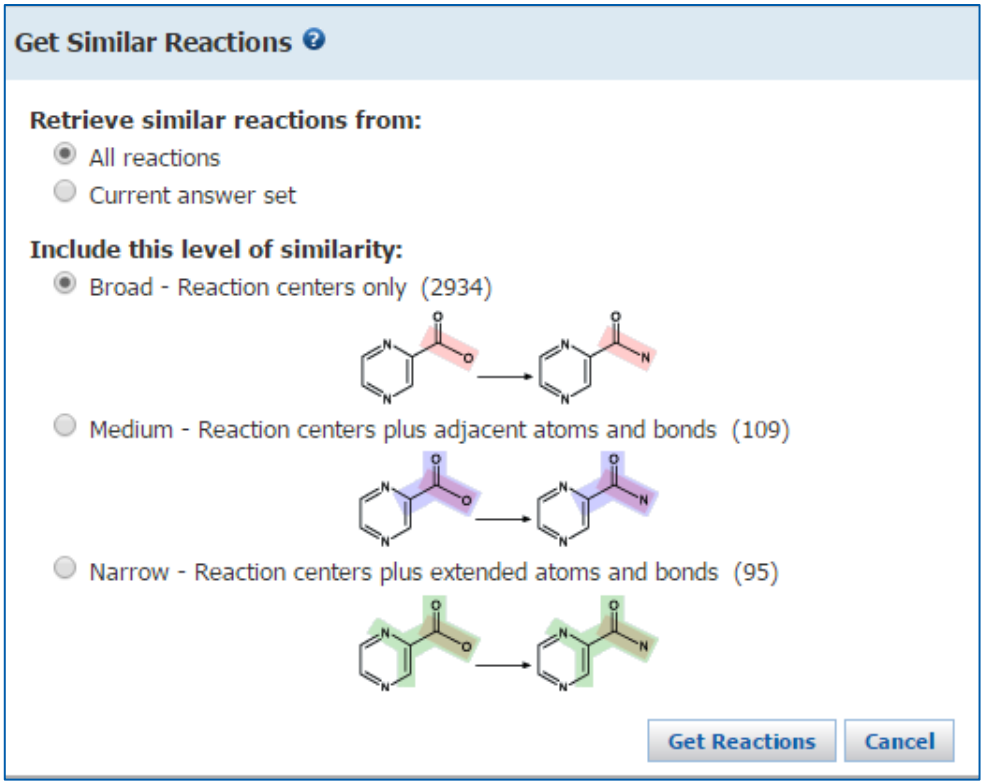
获取相似反应

选择相似反应的相似限制：

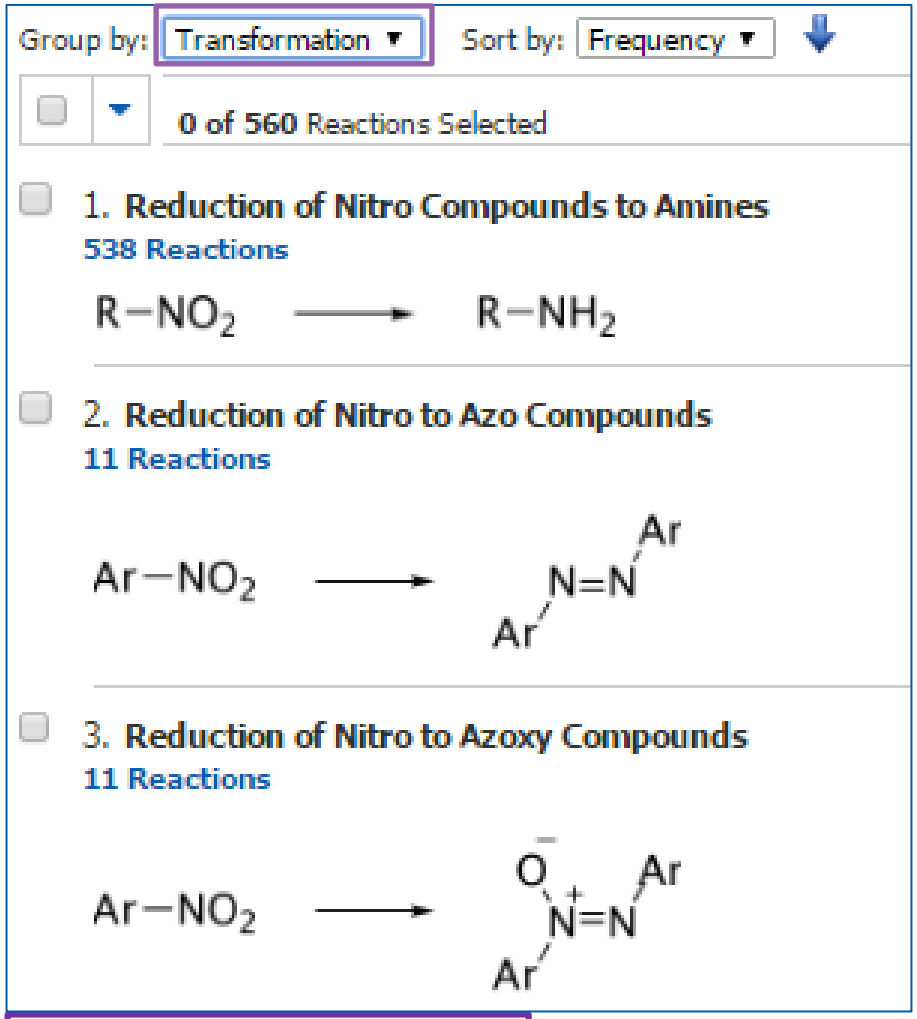
Broad：仅反应中心相似

Miedum：反应中心及附属原子和键

Narrow：反应中心及扩展的原子和键



按照反应类型排序

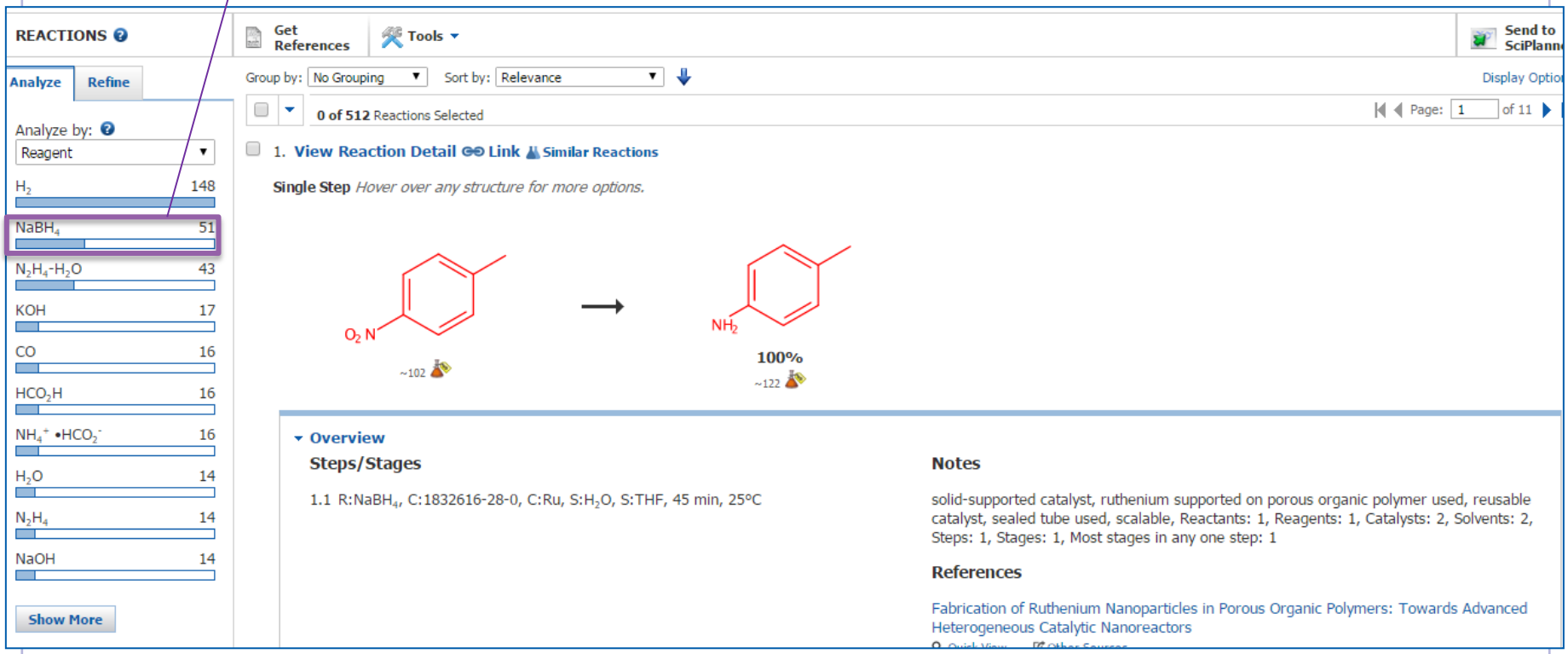


更精确的查找需要的反应

SciFinder® A CAS SOLUTION

反应检索结果的筛选

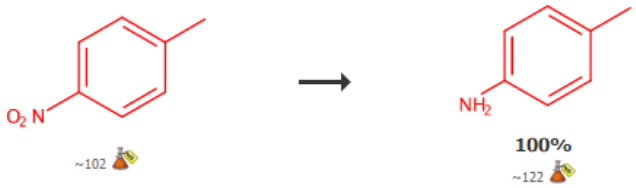
获得特定物质做还原剂的反应



SciFinder® A CAS SOLUTION

SciFinder囊括最大的反应实验过程合集

Single Step *Hover over any structure for more options.*



▾ **Overview**

Steps/Stages

1.1 R:H_2, R:Cs_2CO_3, C:1610424-70-8, C:1034343-98-0 (oxide), S:PhMe, 2 h, 100°C, 1 atm

Notes

solid-supported catalyst, palladium catalyst supported on graphene oxide prepared and used, reusable catalyst, Reactants: 1, Reagents: 2, Catalysts: 2, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References

Catalyst Enhancement and Recyclability by Immobilization of Metal Complexes onto Graphene Surface by Noncovalent Interactions

Quick View Other Sources

By Sabater, Sara et al

From ACS Catalysis, 4(6), 2038-2047; 2014

▾ **Experimental Procedure**

ACS Catalysis

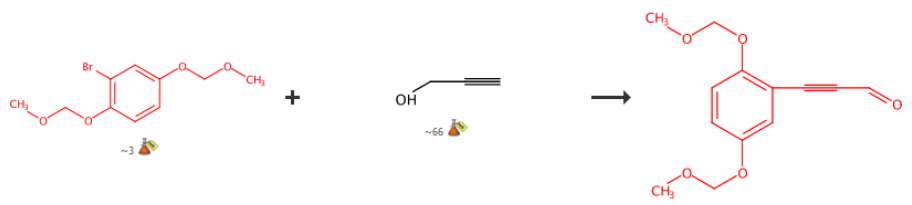
General/Typical Procedure: **General Procedure for Nitroarene Reductions.** Molecular hydrogen was added with a balloon filled with 1 atm of H_2 to a mixture of nitroarene (0.3 mmol), Cs_2CO_3 (0.3 mmol), anisole as internal standard (0.3 mmol), and NHC-Pd-rGO (6×10^{-3} mmol, based on metal) in toluene (5 mL). The system was then evacuated and backfilled with H_2 in cycles for three times before putting the reaction vessel in an oil bath at 100°C for 2h. Yields were determined by GC analyses using anisole (0.3 mmol) as internal standard. Products were identified according to spectroscopic data of the commercially available compounds. Entry: 4; Yield 100%.

不用阅读全文，直接获得包含实验过程的反应记录

SciFinder® A CAS SOLUTION

SciFinder囊括最大的反应实验过程合集

2 Steps *Hover over any structure for more options.*



▾ **Overview**

Steps/Stages

1.1 C:Pd(PPh_3)$_4$, S:$BuNH_2$, 21 h, 100°C
2.1 R:DMSO, R:Cl(O=)CC(=O)Cl, S:CH_2Cl_2, 15 min, -78°C
2.2 S:CH_2Cl_2, -78°C; 2 h, -78°C
2.3 R:Et_3N, 30 min, -78°C; -78°C → rt
2.4 R:H_2O, R:NH_4Cl, 30 min, rt

Notes

1) key step, alternate catalyst concentration, catalyst (CuI) and tem
yield, Sonogashira coupling, 2) key intermediate, Swern oxidation, s
method shown, Reactants: 2, Reagents: 5, Catalysts: 1, Solvents: 2, St
Most stages in any one step: 4

References

Synthesis of Bioactive Speciosins G and P from Hexagonia speciosa
Quick View Other Sources
By Guerrero-Vasquez, Guillermo A. et al
From Journal of Natural Products, 77(9), 2029-2036; 2014

Experimental Procedure:

我们可以做得更好

- 更好的阅读体验?
- 这些数字代表什么？
- 查免费的Supporting Information？可能只有图谱。

▾ **Experimental Procedure**

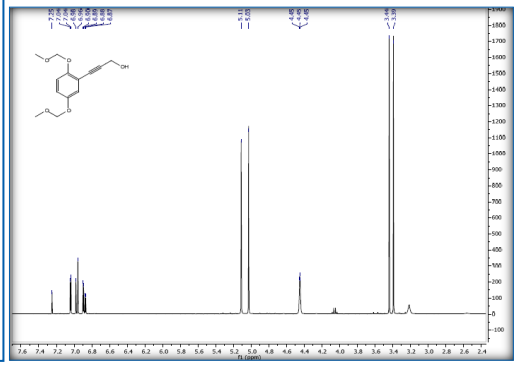
JOURNAL OF NATURAL PRODUCTS

Step 1

General Procedure for the Sonogashira Coupling.[8,10,11] Compounds **6a** [31] and **16** [8] were synthesized according to literature procedures. Aryl halide **6a** or **16** (9.21 mmol) in n-butylamine (6.4 mL) was placed in a flame-dried round-bottomed flask under an argon atmosphere. A mixture of terminal alkynes **7**, **25**, **26**, or **27** (9.21 mmol) in n-butylamine (10 mL) and $Pd(Ph_3)_4$ (5% or 3%) was added, with the optional addition of CuI (3%) where appropriate. The mixture was heated for 21 h at 98 °C and poured intoH_2O(80 mL). The product was extracted with EtOAc (3 × 80 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and evaporated under reduced pressure. The crude product was purified by silica gel column chromatography (EtOAc/hexanes, 10-50%). *3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-yn-1-ol*[F2] (**8**). Yield 96%; colorless oil. IR (KBr) ν_{max} 3310, 2230 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 4.51 (2H, s, H-1a), 5.09 (2H, s, H-4a), 5.17 (2H, s, H-1a), 6.95 (1H, dd, J = 9 and 3.0 Hz, H-5), 7.03 (1H, d, J = 9.0 Hz, H-6), 7.10 (1H, d, J = 3.0 Hz, H-3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 51.81 (C-9), 56.05 (C-4b), 56.38 (C-1b), 81.74 (C-7), 91.56 (C-8), 95.14 (C-4a), 95.88 (C-4b), 114.19 (C-2), 117.13 (C-5), 118.50 (C-3), 121.20 (C-6), 151.95 (C-4), 153.06 (C-1); HRESIMS *m/z* 275.0900 [M + Na]$^+$ (calcd for $C_{13}H_{16}O_5$ 275.0896).

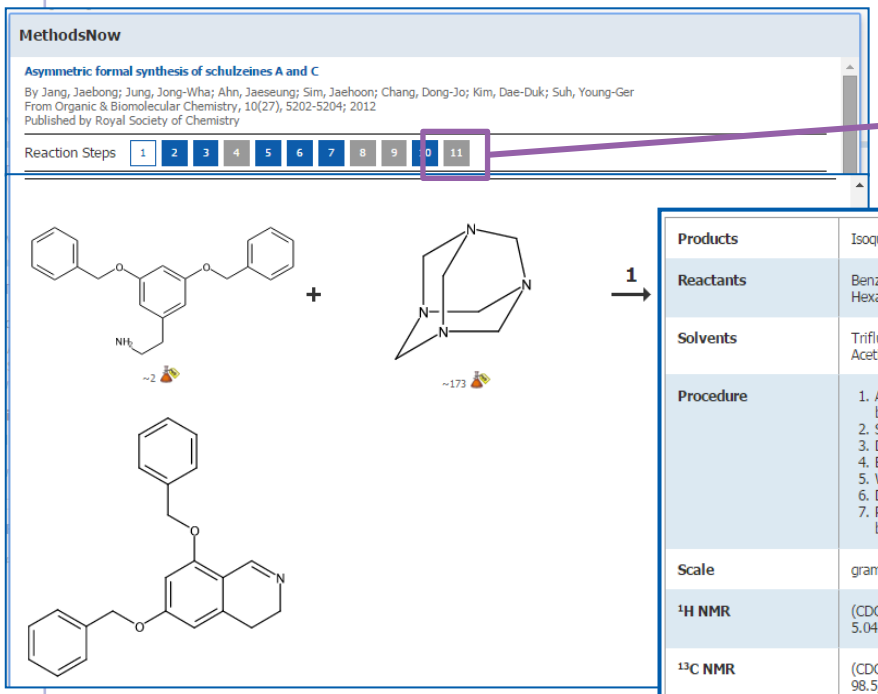
Step 2

Generation of the Key Aldehyde.[17] Oxalyl chloride (272.3 μL, 3.12 mmol) in dry CH_2Cl_2 (9 mL) was added to a stirred solution of DMSO (332 μL, 4.68 mmol) in dry CH_2Cl_2 (1.5 mL) under an argon atmosphere at -78 °C. The mixture was stirred for 15 min, and the alcohol 8 (393.5 mg, 1.56 mmol) or alcohol **17** (300 mg, 1.56 mmol) in dry CH_2Cl_2 (12 mL) was added dropwise (Note: Swern oxidation could be scaled-up to 1.56 mmol of starting material). After the starting material had been consumed (nearly 2 h), Et_3N (1.88 mL, 7.8 mmol) was added. The reaction mixture was stirred at -78 °C for a further 30 min and was allowed to warm to rt and quenched with saturated NH_4Cl and H_2O, and the mixture was stirred for 30 min. The organic phase was decanted off, and the aqueous layer was extracted with CH_2Cl_2 (3 × 30 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, and evaporated under reduced pressure. *3-[2,5-Bis(methoxymethoxy)phenyl]prop-2-ynal* (**9**). Yield 91%; colorless oil. IR (KBr) ν_{max} 1660, 2194 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 3.46 (3H, s, H-4b), 3.51 (3H, s, H-1b), 5.10 (2H, s, H-4a), 5.21 (2H, s, H-1a), 7.09 (1H, dd, J = 9.2 and 1.2 Hz, H-6), 7.12 (1H, dd, J = 9.1 and 2.2 Hz, H-5), 7.22 (1H, dd, J = 2.2 and 1.3 Hz, H-3), 9.44 (1H, s, H-9); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 56.18 (C-4b), 56.54 (C-1b), 92.05 (C-8), 92.27 (C-7), 95.22 (C-4a), 95.58 (C-1a), 110.70 (C-2), 116.72 (C-6), 122.0 (C-5), 122.09 (C-3), 151.85 (C-4), 154.88 (C-1), 176.92 (C-9); HRESIMS *m/z* 273.0741 [M + Na]$^+$ (calcd for $C_{13}H_{14}O_5$ 273.0739).



SciFinder® A CAS SOLUTION

MethodsNow Synthesis



多步反应中，原文没有描述的实验过程以灰色标示

Products	Isoquinoline, 3,4-dihydro-6,8-bis(phenylmethoxy)-, 95%, CAS RN: 1384461-35-1
Reactants	Benzeneethanamine, 3,5-bis(phenylmethoxy)-, CAS RN: 188662-05-7 Hexamethylenetetramine, CAS RN: 100-97-0
Solvents	Trifluoroacetic acid, CAS RN: 76-05-1 Acetic acid, CAS RN: 64-19-7
Procedure	1. Add hexamethylenetetramine (3.1 g, 22.1 mmol) to the mixture of 2-(3,5-bis(benzyloxy)phenyl)ethylamine (2.0 g, 11.0 mmol), AcOH (12 mL) and TFA (3 mL) under argon 2. Stir the mixture for 3hours at 90ÊC. 3. Dilute the reaction mixture with H_2O. 4. Basify with potassium carbonate and extract with CH_2Cl_2. 5. Wash the combined organic layers with brine. 6. Dry over $MgSO_4$ and concentrate in vacuo. 7. Purify the residue by column chromatography on silica gel (5 to 10% EtOAc in hexane) to obtain 6,8-bis(benzyloxy)-3,4-dihydroisoquinoline.
Scale	gram
^{1}H NMR	($CDCl_3$, 400 MHz) δ 8.69 (s, 1H), 7.43 - 7.29 (m, 10H), 6.45 (d, *J* = 1.88 Hz, 2H), 6.36 (s, 1H), 5.05 (s, 2H), 5.04 (s, 2H), 3.67 (t, 2H), 2.65 (t, 2H)
^{13}C NMR	($CDCl_3$, 100 MHz) δ 161.9, 157.7, 155.2, 140.0, 136.3, 128.6, 128.5, 128.1, 128.0, 127.4, 127.1, 111.9, 105.3, 98.5, 70.1, 46.5, 26.0
IR	(thin film, neat) ν_{max} 3062, 3032, 2935, 1736, 1620, 1603, 1575, 1497, 1442, 1377, 1351, 1309 cm^{-1}
HRMS	(FAB+) calcd for $C_{23}H_{22}NO_2$ (M+H$^+$) 344.1651; found 344.1658
Mass Spec	(FAB+) *m/z* 344 (M+H$^+$)
State	yellow solid
CAS Method Number	3-614-CAS-200055

Print/Export Close

物质信息

实验过程

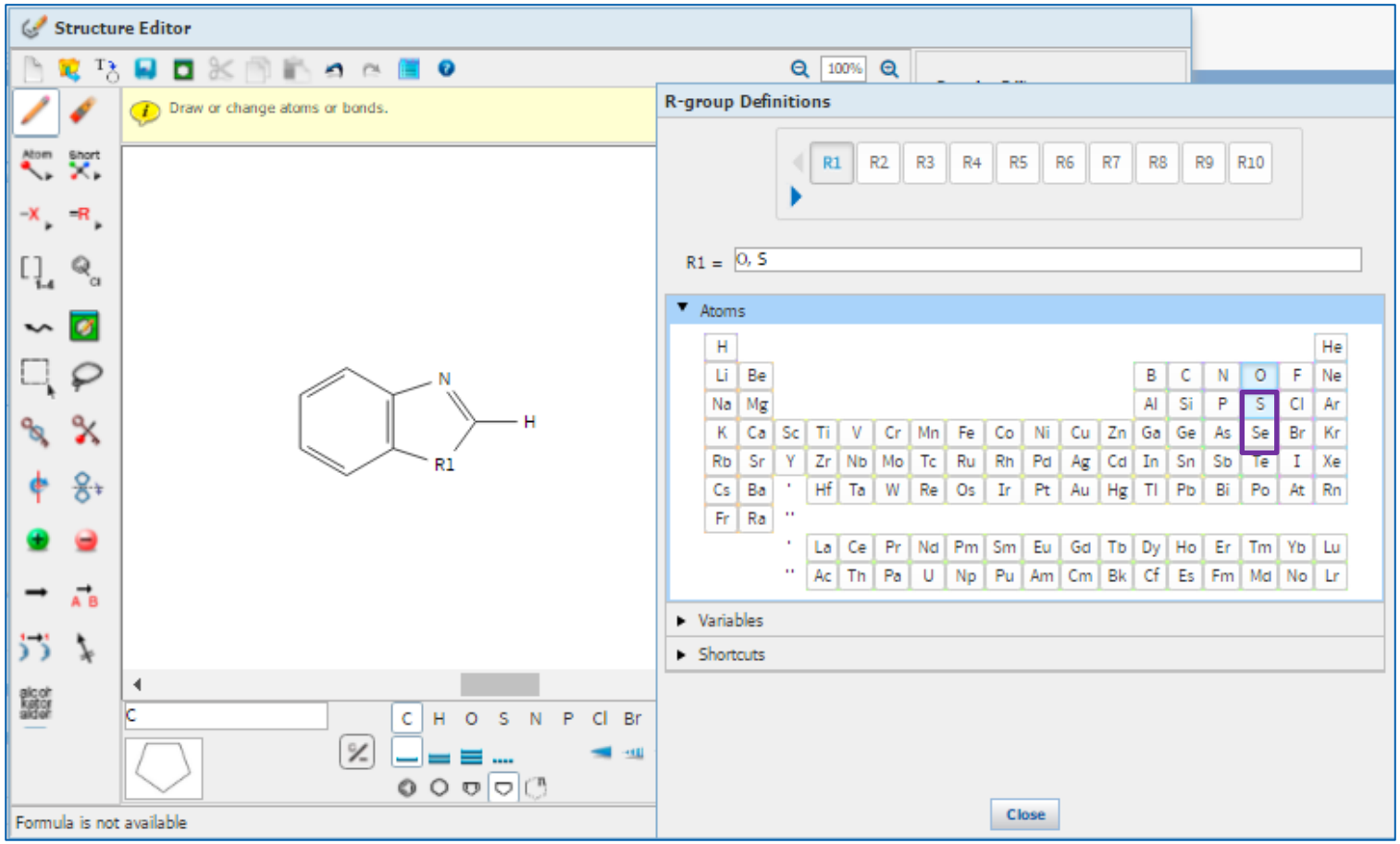
图谱信息

保存/导出方法

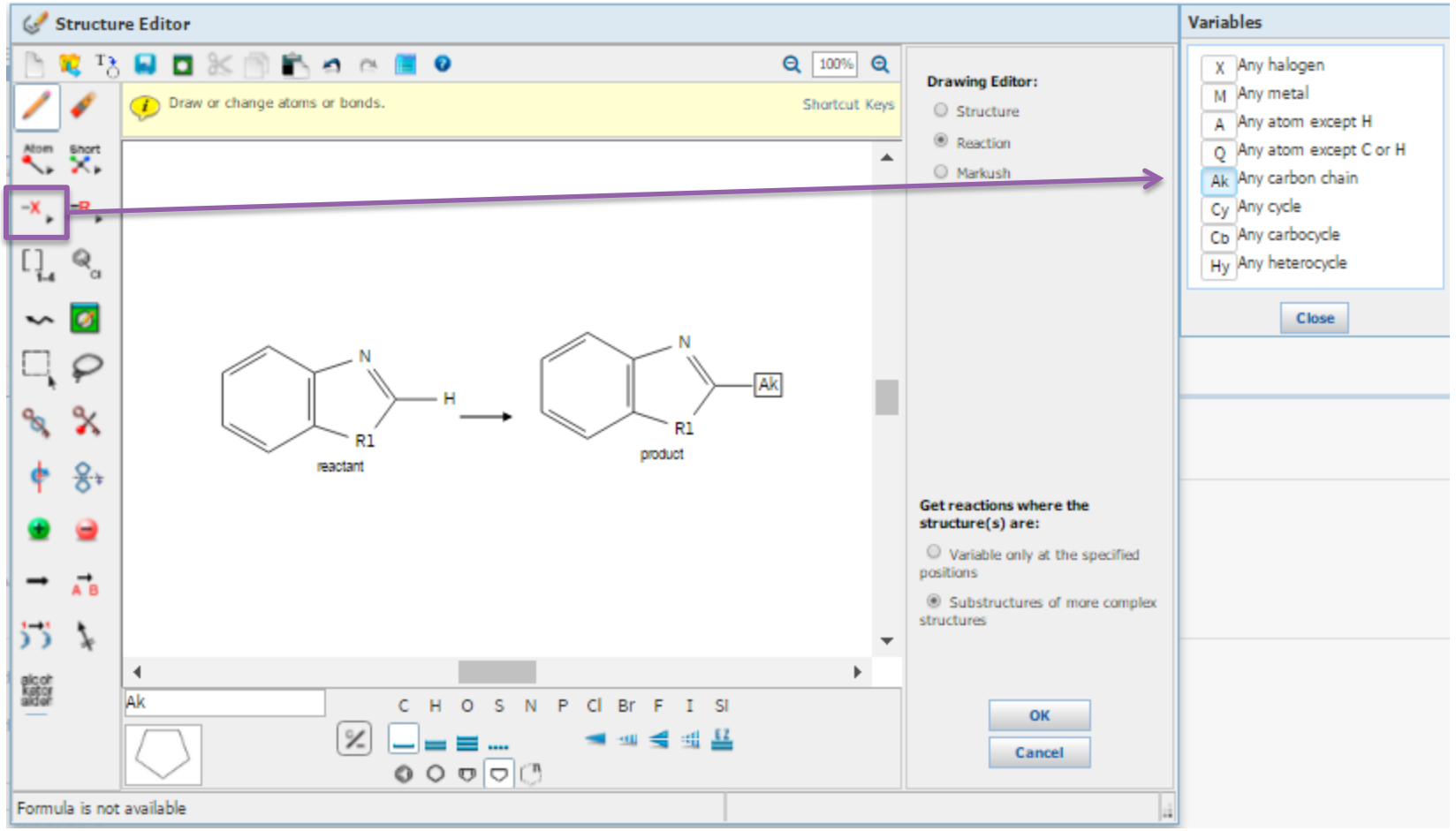
SciFinder® A CAS SOLUTION

亚结构反应检索

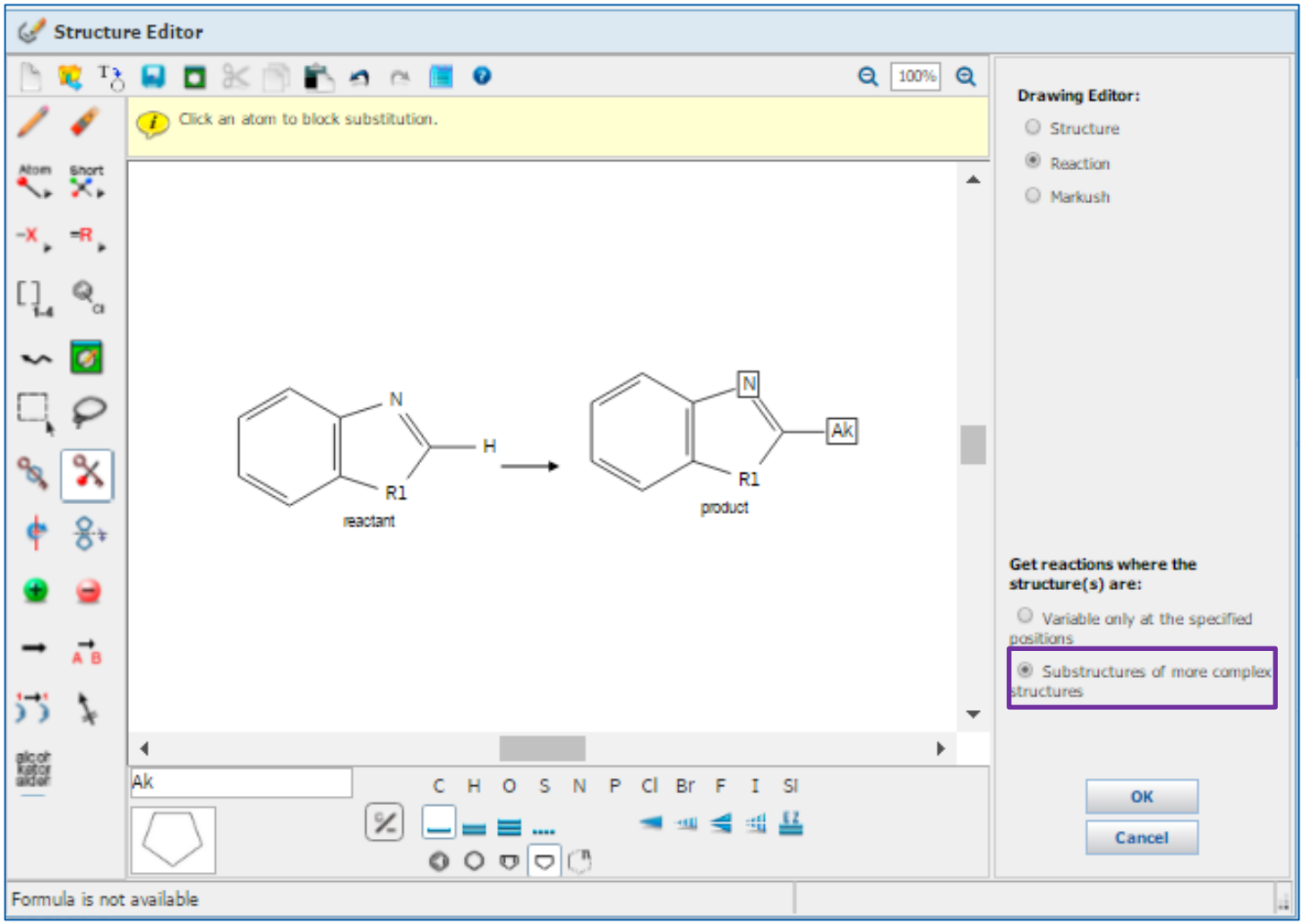
通过C-H活化对苯并噻唑或者恶唑进行烷基化



亚结构反应检索


Structure Editor
Draw or change atoms or bonds.
Shortcut Keys
100%
Drawing Editor:
Structure
Reaction
Markush
N
H
R1
reactant
N
Ak
R1
product
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
Ak
C H O S N P Cl Br F I Si
OK
Cancel
Formula is not available
Variables
X Any halogen
M Any metal
A Any atom except H
Q Any atom except C or H
Ak Any carbon chain
Cy Any cycle
Cb Any carbocycle
Hy Any heterocycle
Close

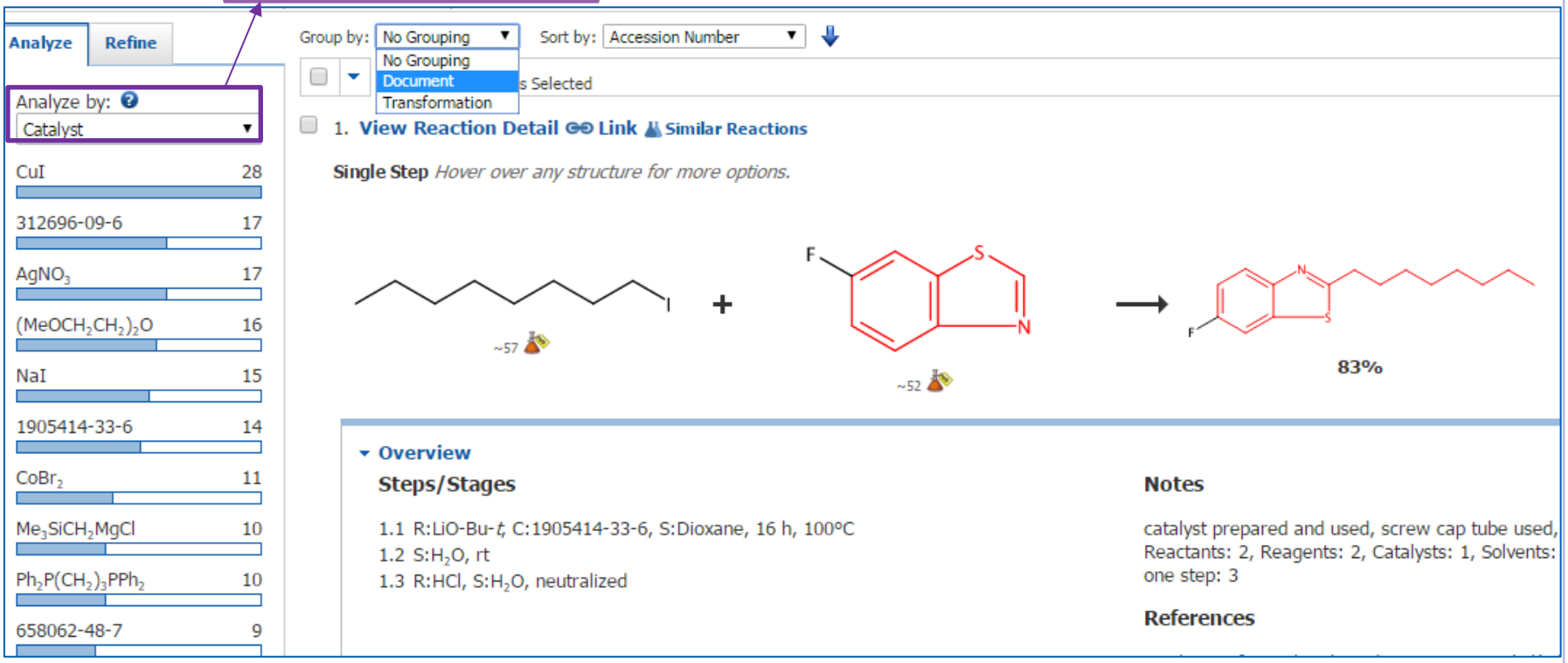
亚结构反应检索



SciFinder® A CAS SOLUTION

通过后处理工具筛选反应--Analyze

通过催化剂筛选反应



SciFinder® A CAS SOLUTION

提纲

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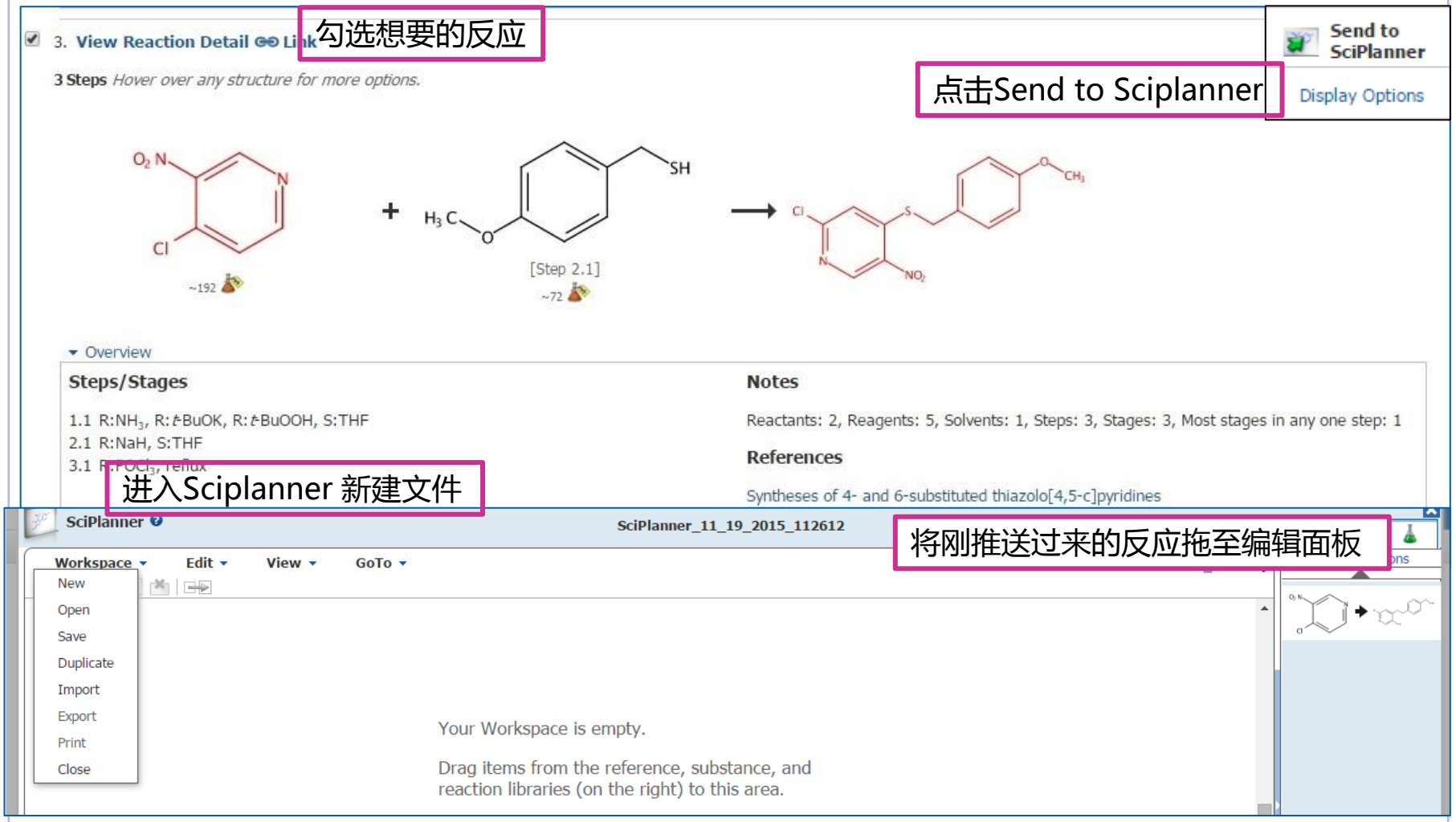
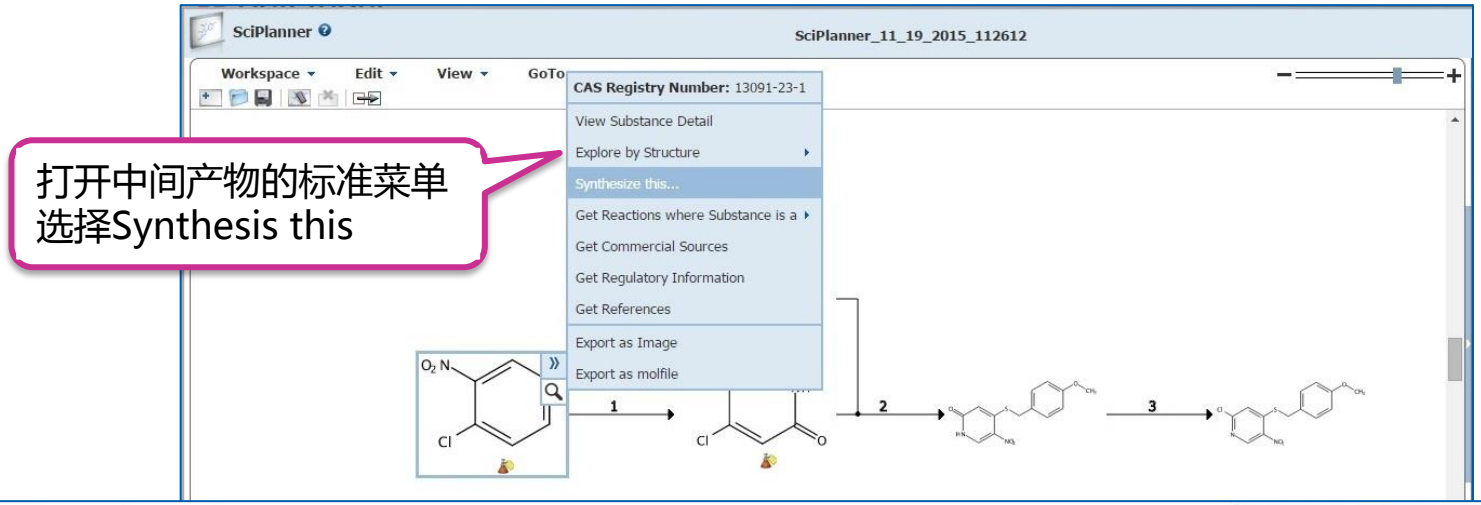
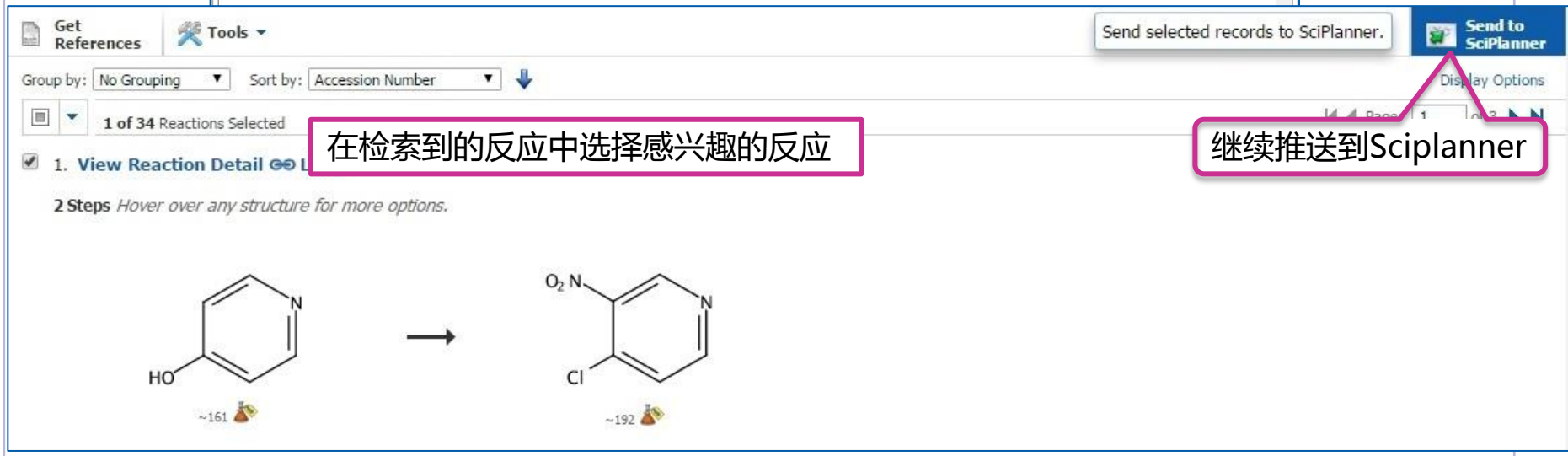
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

SciPlanner使用简介

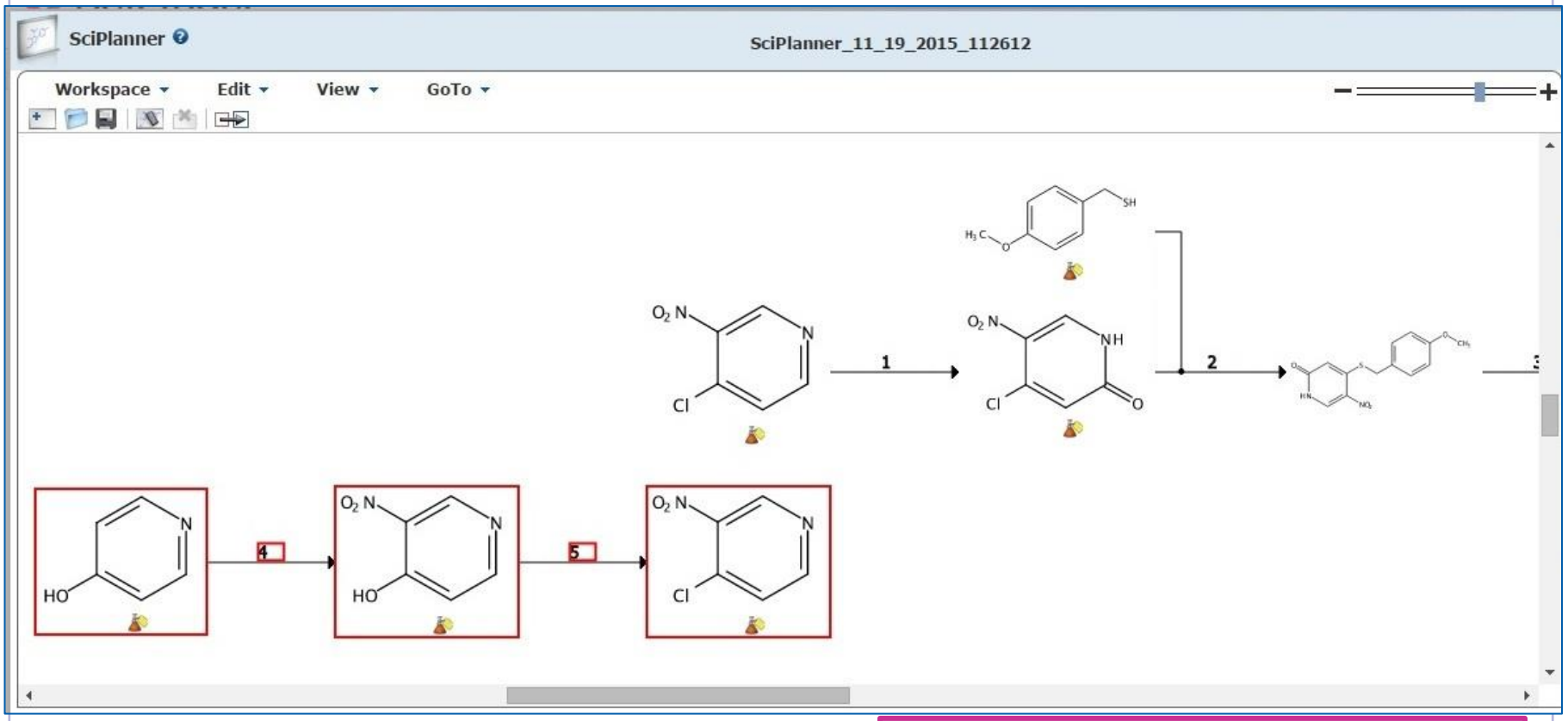


SciPlanner使用简介



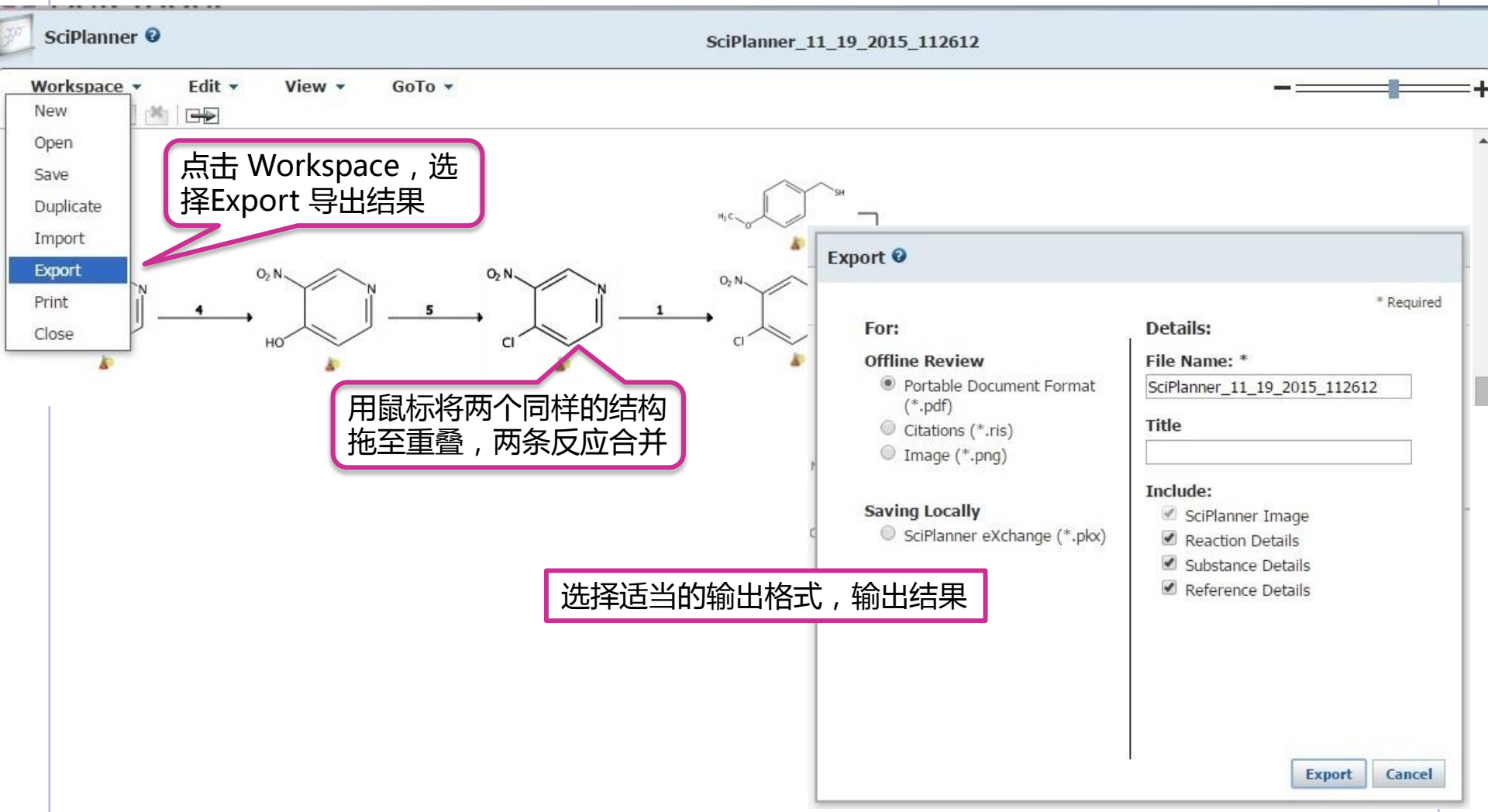


SciPlanner使用简介



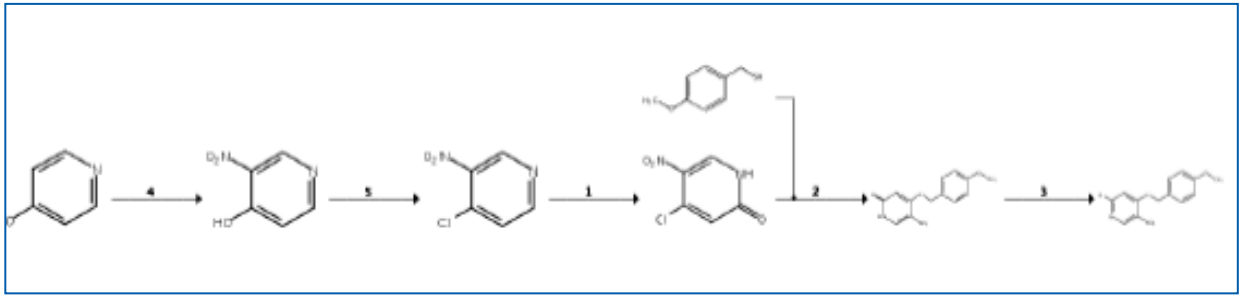
步骤同前，将推送过来的反应拖到编辑面板中，可以看到两条反应中存在同样的结构

SciPlanner使用简介



SciFinder® A CAS SOLUTION

SciPlanner导出结果



Reaction	Stages		Notes	Yield
5	1.1	R:$POCl_3$, S:PhMe, 0°C → rt; 16 h, rt → 110°C	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	90%
	1.2	R:K_2CO_3, S:H_2O, cooled, pH 10	**Transformation:** 1. Formation of Alkyl Halides from Alcohols	

References

High color rendering index and color stable hybrid white efficient OLEDs with a double emitting layer structure using a single phosphorescence dopant of heteroleptic platinum complexes

By Poloek, Anurach et al

From Journal of Materials Chemistry C: Materials for Optical and Electronic Devices, 2(48), 10343-10356; 2014

Substance Information

1228150-22-8 $C_{13}H_{12}N_2O_4S$ 2(1*H*)-Pyridinone, 4-[[(4-methoxyphenyl)methyl]thio]-5-nitro- **Related Info:** ~ 2 References Reactions	**1228150-23-9** $C_{13}H_{11}ClN_2O_3S$ Pyridine, 2-chloro-4-[[(4-methoxyphenyl)methyl]thio]-5-nitro- **Related Info:** ~ 2 References Reactions	**13091-23-1** $C_5H_3ClN_2O_2$ Pyridine, 4-chloro-3-nitro- **Related Info:** ~ 391 References Reactions ~ 190 Commercial Sources Regulatory Information
5435-54-1 $C_5H_4N_2O_3$ 4-Pyridinol, 3-nitro- **Related Info:** ~ 113 References Reactions ~ 197 Commercial Sources Regulatory Information	**6258-60-2** $C_8H_{10}OS$ Benzenemethanethiol, 4-methoxy- **Related Info:** ~ 749 References Reactions ~ 71 Commercial Sources Regulatory Information	**626-64-2** C_5H_5NO 4-Pyridinol **Related Info:** ~ 1351 References Reactions ~ 160 Commercial Sources Regulatory Information
850663-54-6 $C_5H_3ClN_2O_3$ 2(1*H*)-Pyridinone, 4-chloro-5-nitro- **Related Info:** ~ 22 References Reactions ~ 136 Commercial Sources		

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提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
  - Markush检索
  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

MethodsNowTM 是一个完整的 CAS 解决方案

- 最大的方法信息合集，聚焦核心化学市场
- 来自重要的全文信息资源：CAS高质量标引、全新的、增值的方法
- 满足合成和分析研究工作者的需求
- 分析与合成两个模块
- 逾百万的合成和分析方法合集——数量持续增加!

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MethodsNow – Analysis(www.methodsnow.com)

- Organic Compound Analysis: 天然产物分离分析，手性分离，活性药物成分及代谢产物分析…
- Organometallics / Inorganics: 地质分析，无机物分析，金属有机化合物分析
- Pharmacology / Toxicology: 成瘾药物检测，有毒物检测…
- Bioassays: 生物探针，生物标定细胞实验，生物标定药物实验，生物医学材料分析，生物分子/生物组织分离测定…
- Water Analysis: 阴阳离子分析，元素测定，痕量元素分析，废水分析，生物标记公共卫生分析…
- Historical Analysis / Dating: 考古分析，同位素分析
- Environmental Analysis: 土壤/空气/水分析，农药残留分析…
- Agricultural Applications / Analysis: 除草剂分析…
- Food Analysis: 脂肪酸分析，脂肪酸酯分析，蛋白质分析…
- Fuels / Geology / Biofuels: 生物燃料分析，油气分析，石油产品分析，煤炭加工…
- Miscellaneous: 化妆品分析，爆炸物分析，纳米材料分析…

目前有13个大类，45个小类。某些子项目属于多种方法分类

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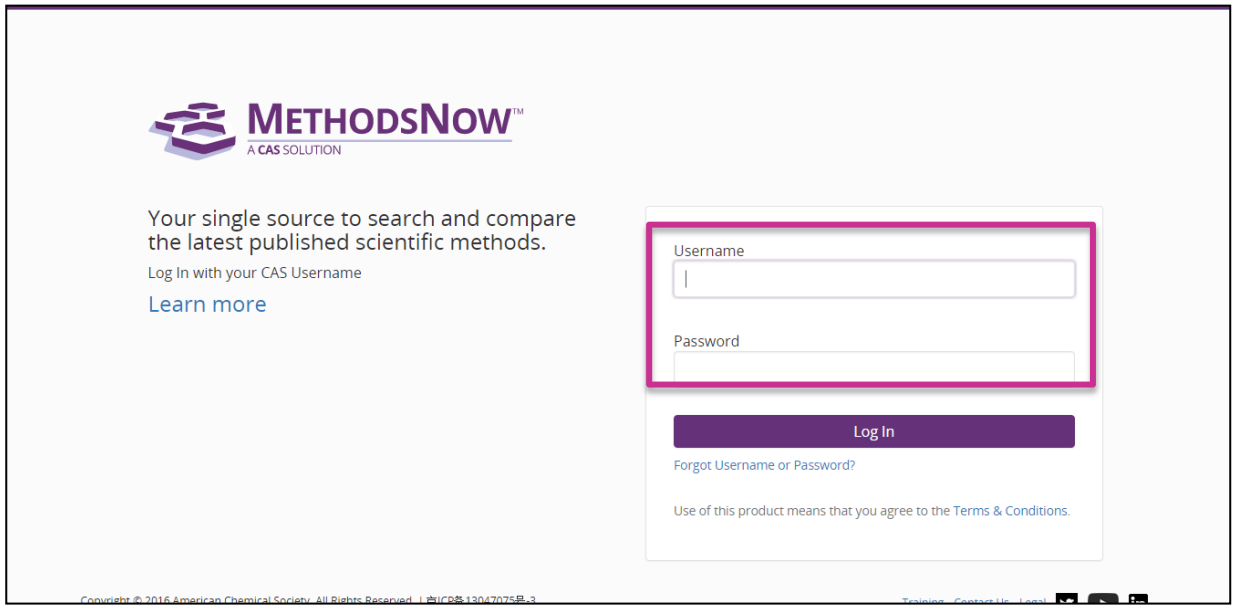

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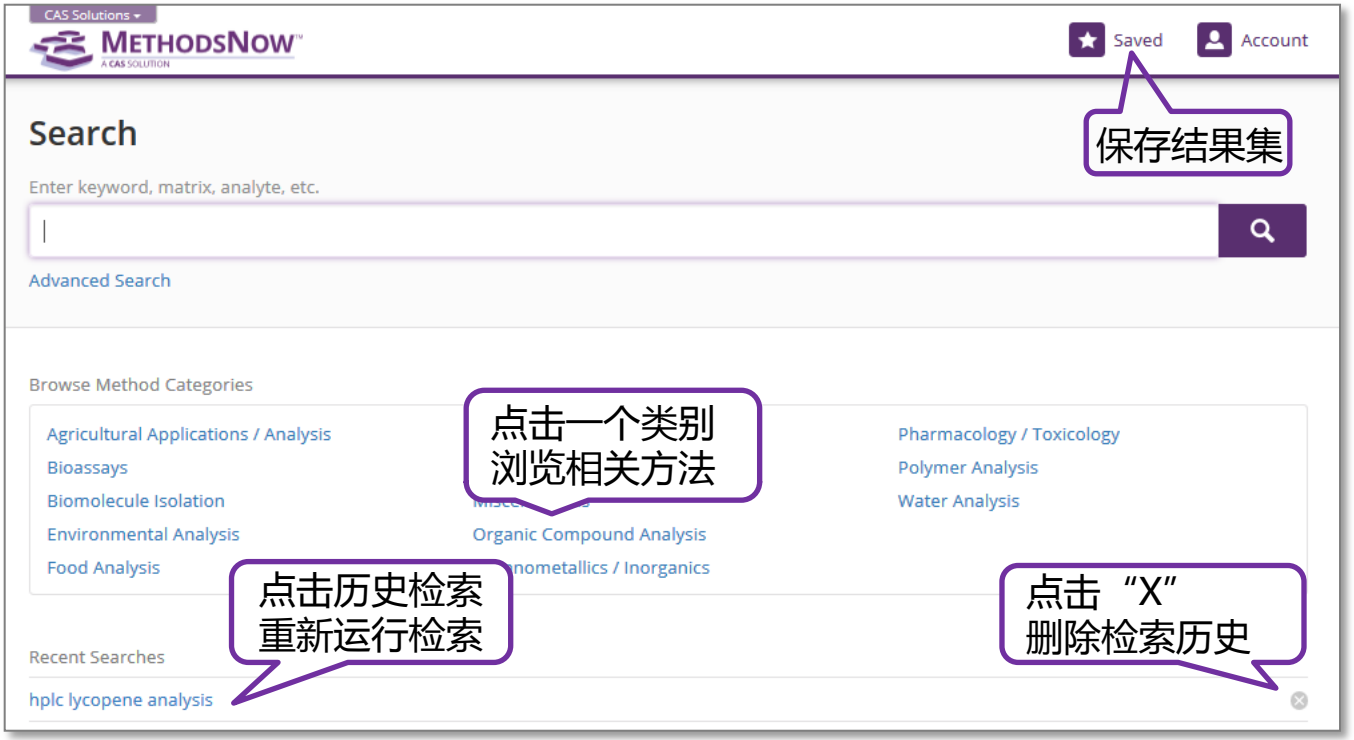
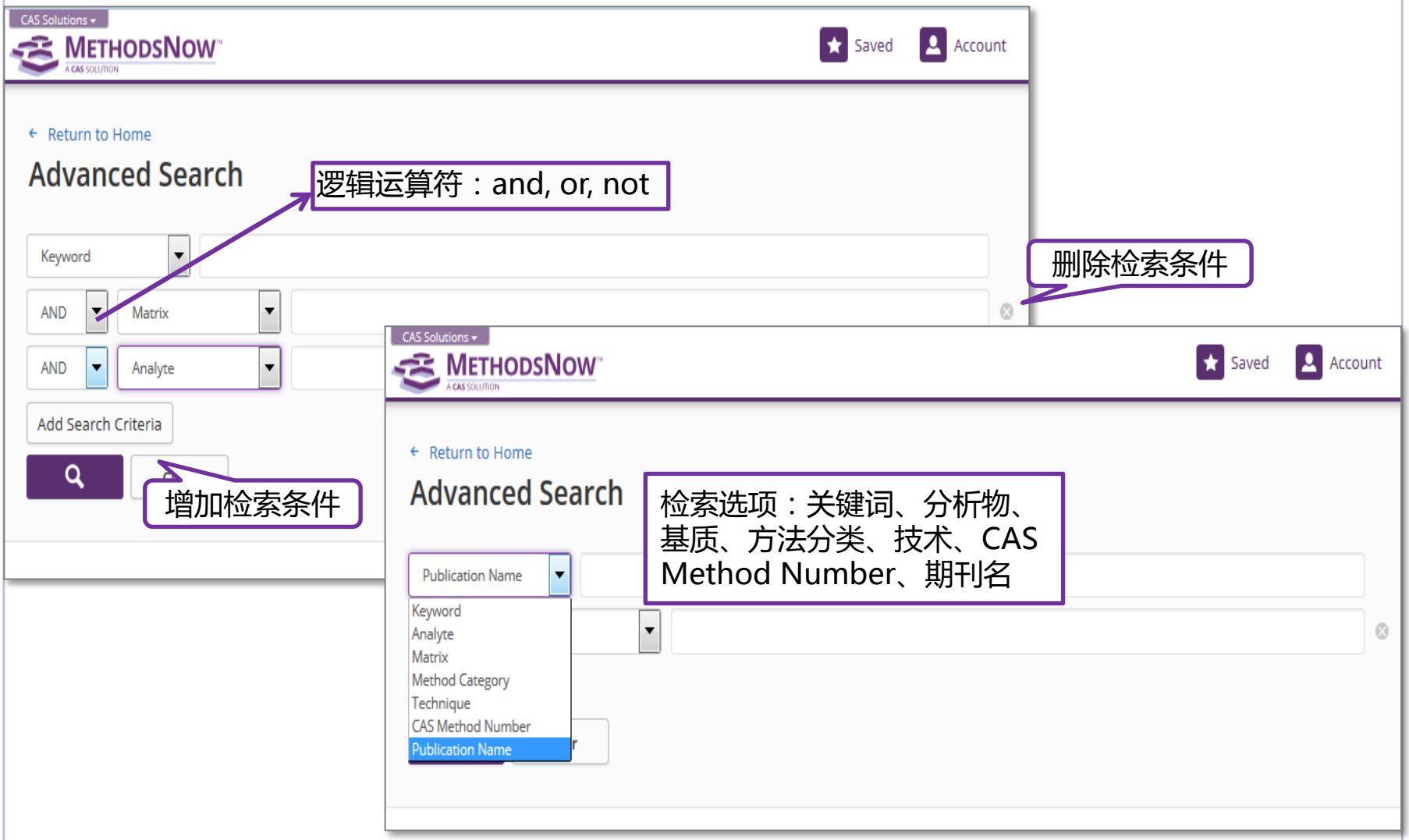
检索/高级检索

方法分类

历史检索



高级检索



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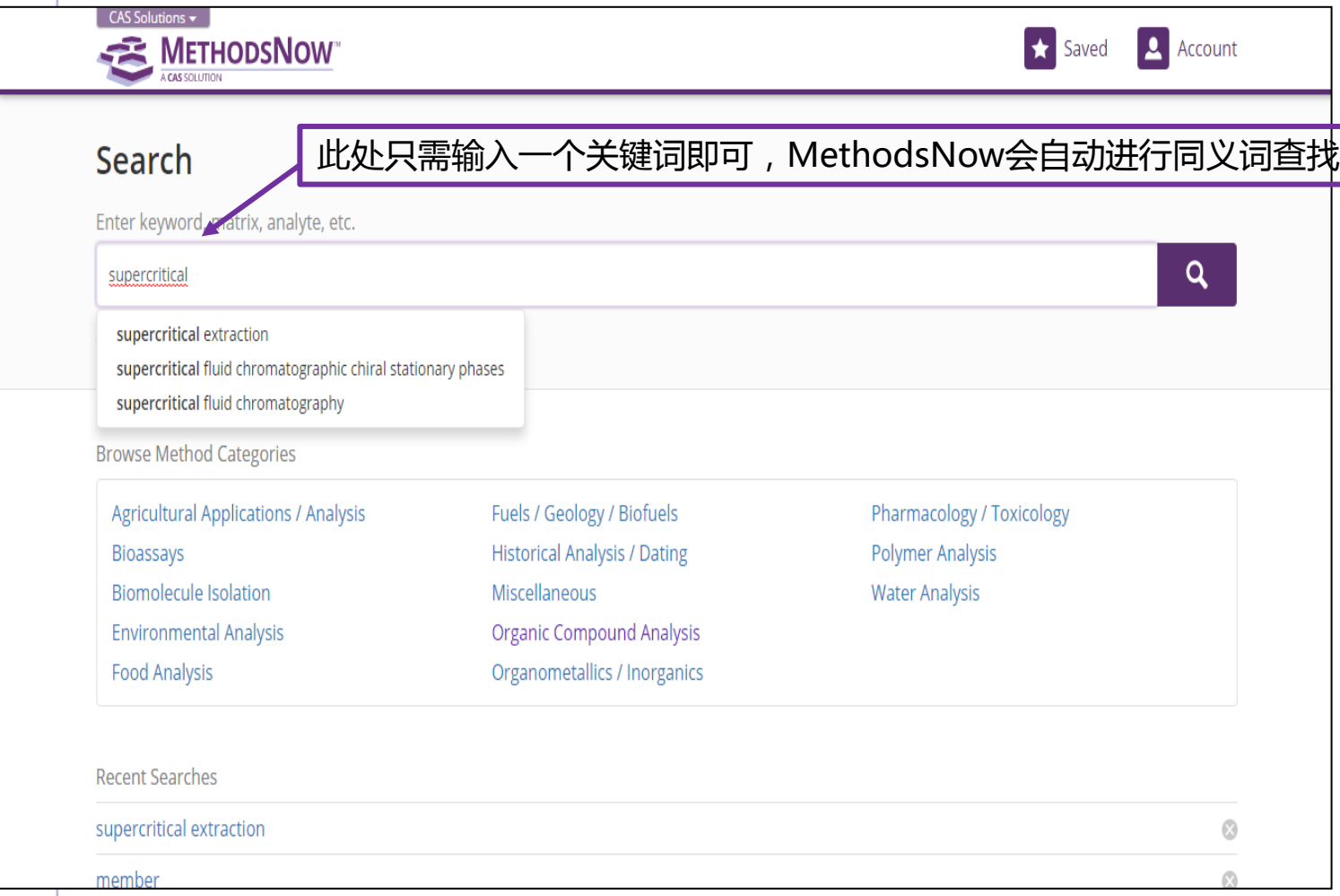
案例：利用超临界萃取法分析叶片中的酚类物质



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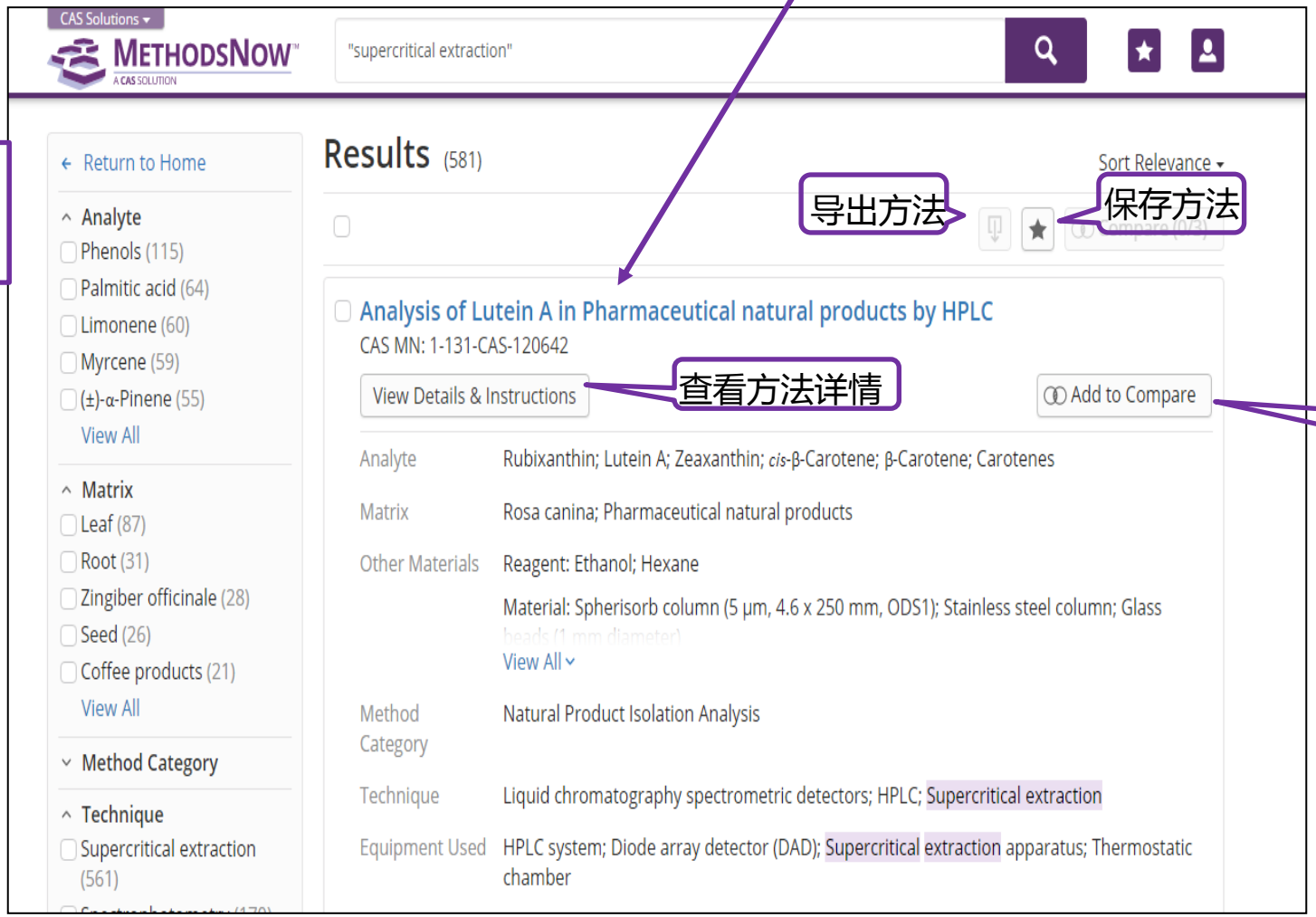
结果显示

典型分析方法标题格式：通过某技术手段在某基质中分析某物质

限定分析物、基质、方法等条件



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结果显示

Analysis of Phenols in Calophyllum brasiliense by Supercritical extraction

CAS MN: 2-105-CAS-52171

Method Category: Antioxidant Assay
Technique: Spectrophotometry; Soxhlet extractor; Supercritical extraction

Materials	Role	Image	CAS RN
Mammea A/BB	analyte	View Structure	6916-62-7
Xanthone	analyte	View Structure	90-47-1
Coumarin	analyte	View Structure	91-64-5
Phenols	analyte		
Biflavonoids	analyte		
Calophyllum brasiliense	matrix		
Leaf	matrix		
Sieves (30 and 50 mesh)	material		
Dichloromethane	reagent	View Structure	75-09-2
Methanol	reagent	View Structure	67-56-1
DPPH radical	reagent	View Structure	1898-66-4

实验材料

Source

Comparing conventional and supercritical extraction of (-)-mammea A/BB and the antioxidant activity of Calophyllum brasiliense extracts

Goncalves, Renata Menoci; Lemos, Caroline Ortega Terra; Leal, Ivana Correa Ramos; Nakamura, Celso Vataru; Cortez, Diogenes Aparicio Garcia; da Silva, Edson Antonio; Cabral, Vladimir Ferreira; Cardozo-Filho, Lucio

Molecules (2013), 18, 6215 - 6229. MDPI AG

CODEN: MOLEFW | ISSN: 14203049 | DOI: 10.3390/molecules18066215

Document Sources

Abstract ^

Calophyllum brasiliense is a rich source of bioactive coumarins, xanthones and biflavonoids. The aim of the study was to compare the phenol contents and the antioxidant activity of C. brasiliense extracts obtained by conventional and supercritical fluid extraction (SFE) methods, as well as the quantification of crude extracts and (-)-mammea A/BB yields. Dichloromethane and hexane were used as solvents for the conventional extractions and SFE was developed using supercritical CO_2; the kinetic curves were modeled using a second-order empirical model. The dichloromethane extract presented the best total yield, although it showed the lowest content of (-)-mammea A/BB. The concentration of the coumarin was considerably higher in

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文献信息

Instructions

Organic solvent extraction using Soxhlet apparatus

1. Collect the leaves of *Calophyllum brasiliense* Cambess.
2. Dry the plant material in a circulating air oven (QUIMIS Q-31) at 313 K temperature.
3. Mill the leaves in a home processor (WALITA RI7625) after 72 h.
4. Use tyler sieves (W. S. Tyler, Mentor, OH, USA) to classify the samples according to particle size.
5. Select the leaves trapped in the 30 and 50 mesh sieves for the extraction.
6. Perform the organic solvent extraction for 300 min using a Soxhlet apparatus.
7. Use dichloromethane as a solvent due to the differences in terms of polarity and dielectric constant.
8. Set the boiling point at 313 K and the dielectric constant at 8.93.
9. Express the yields obtained for each solvent extraction and calculate in relation to the initial dry weight sample.

Determination of antioxidant activity by DPPH (2,2-diphenyl-1-picrylhydrazyl) method

1. Dilute the extracts in methanol up to concentrations from 25 to 350 µg/mL.
2. Add 2,850 µl of the DPPH solution (0.6 mM) to 150 µL of sample.
3. Substitute the volume of the samples by distilled water for the blank control.
4. Keep the reaction for 1 h at room temperature, in the dark.
5. Measure the absorbance at 515 nm.
6. Express the antioxidant activity (AA%) as a percentage of DPPH radical elimination, calculate according to the following equation: AA% = [(1 – A.sample)/A.blank] × 100, where A.blank represents the absorbance of the blank and A.sample represents the absorbance of the extract solution.
7. Calculate the concentration of the extracts resulting in 50% of inhibition (IC_{50}) from the inhibition percentage plotting graph.

Validation

Inhibitory Activity	206.58 µg/mL (IC_{50})

实验步骤及数据有效性

Equipment Used

Oven, Q-31, QUIMIS

Processor, RI7625, WALITA

Spectrophotometer, UV-1203, Shimadzu

Conditions

Instrument

Detection wavelength - 515 nm

设备条件

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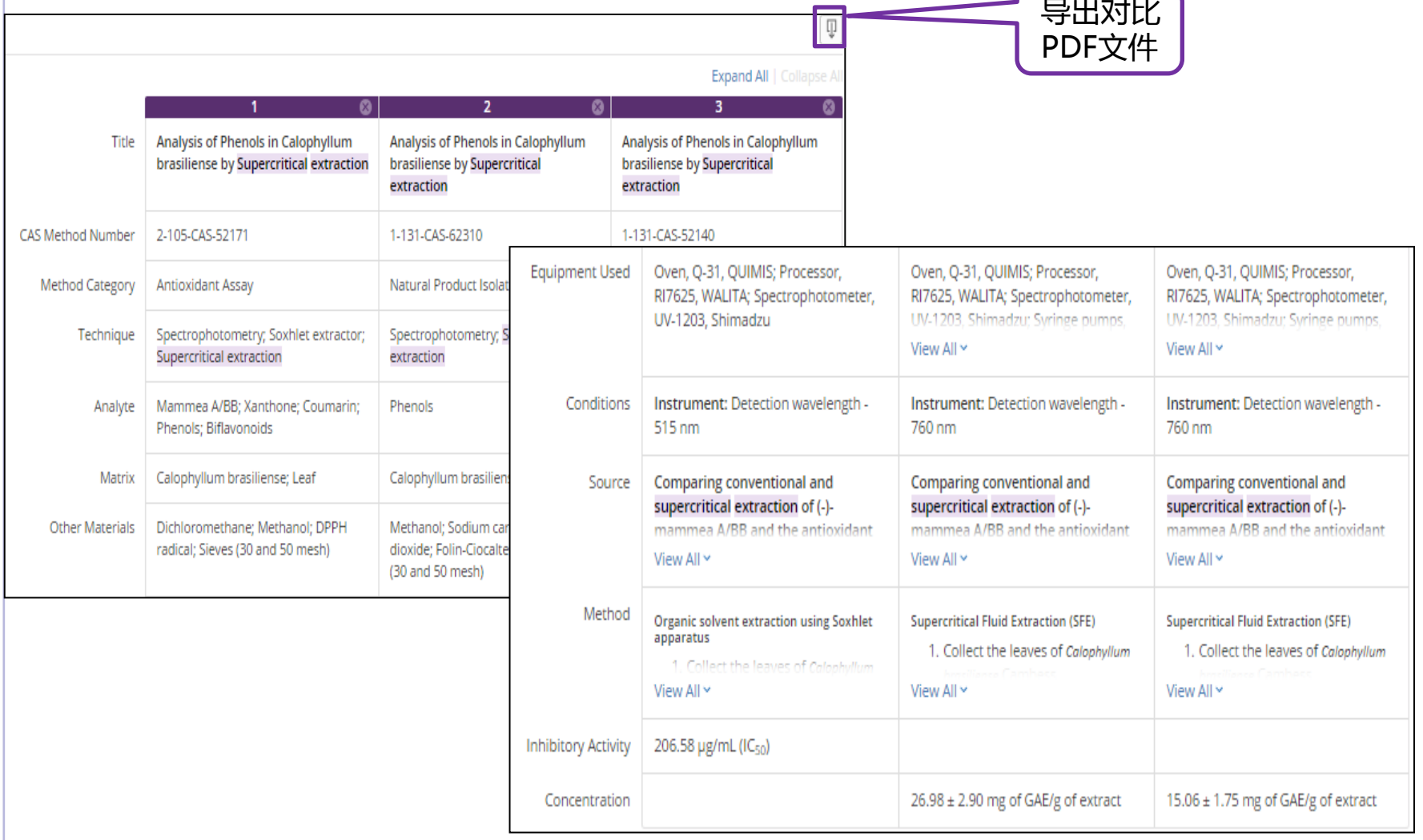
对比不同分析方法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2
3
Title
Analysis of Phenols in Calophyllum brasiliense by Supercritical extraction
Analysis of Phenols in Calophyllum brasiliense by Supercritical extraction
Analysis of Phenols in Calophyllum brasiliense by Supercritical extraction
CAS Method Number
2-105-CAS-52171
1-131-CAS-62310
1-131-CAS-52140
Method Category
Antioxidant Assay
Natural Product Isolat
Technique
Spectrophotometry; Soxhlet extractor; Supercritical extraction
Spectrophotometry; S extraction
Analyte
Mammea A/BB; Xanthone; Coumarin; Phenols; Biflavonoids
Phenols
Matrix
Calophyllum brasiliense; Leaf
Calophyllum brasilien
Other Materials
Dichloromethane; Methanol; DPPH radical; Sieves (30 and 50 mesh)
Methanol; Sodium car dioxide; Folin-Ciocalte (30 and 50 mesh)
Equipment Used
Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu
Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps
View All
Oven, Q-31, QUIMIS; Processor, RI7625, WALITA; Spectrophotometer, UV-1203, Shimadzu; Syringe pumps
View All
Conditions
Instrument: Detection wavelength - 515 nm
Instrument: Detection wavelength - 760 nm
Instrument: Detection wavelength - 760 nm
Source
Comparing conventional and supercritical extraction of (-)-
mammea A/BB and the antioxidant
View All
Comparing conventional and supercritical extraction of (-)-
mammea A/BB and the antioxidant
View All
Comparing conventional and supercritical extraction of (-)-
mammea A/BB and the antioxidant
View All
Method
Organic solvent extraction using Soxhlet apparatus
1. Collect the leaves of Calophyllum
View All
Supercritical Fluid Extraction (SFE)
1. Collect the leaves of Calophyllum
View All
Supercritical Fluid Extraction (SFE)
1. Collect the leaves of Calophyllum
View All
Inhibitory Activity
206.58 µg/mL (IC_{50})
Concentration
26.98 ± 2.90 mg of GAE/g of extract
15.06 ± 1.75 mg of GAE/g of extract

提纲

- 美国化学文摘社简介
- SciFinder简介及检索方式
  - 文献检索
  - 物质检索
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  - 反应检索（MethodsNow Synthesis）
  - SciPlanner
  - MethodsNow
- SciFinder常见问题及解决

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SciFinder浏览器选择建议

- Windows 7以上用户建议升级IE到10以上
- Chrome和FireFox浏览器在所有系统上的表现都优于IE浏览器
- 不建议使用360浏览器检索SciFinder，会被自动拦截相关功能或插件

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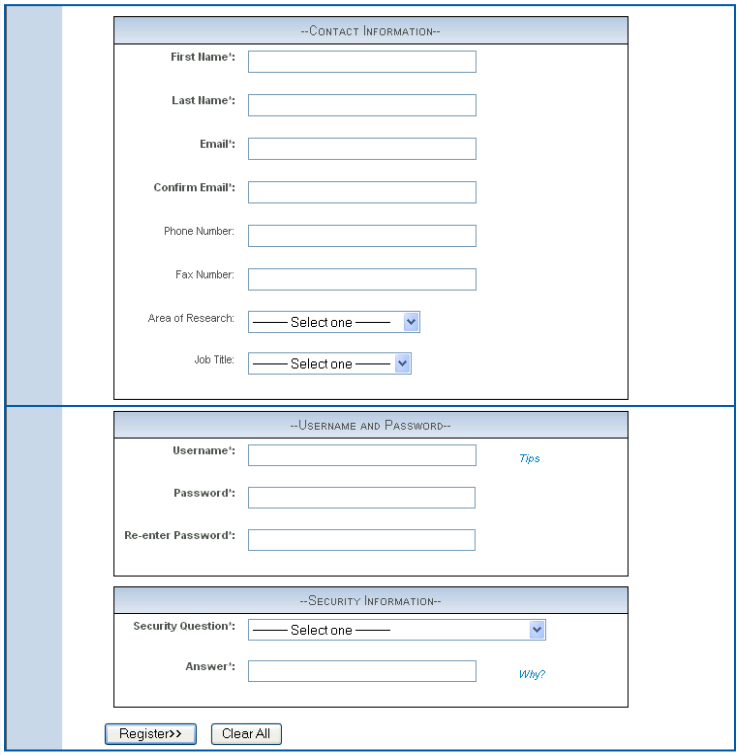

请注意：
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- -（破折号）
- _（下划线）
- .(句点）
- @（表示“at”的符号）

3.密码必须包含 7-15 个字符，并且至少包含三种以下字符：

- 字母
- 混合的大小写字母
- 数字
- 非字母数字的字符（例如 @、#、%、&、*）

例：abc@123
4.从下拉列表中选择一个密码提示问题并给出答案。
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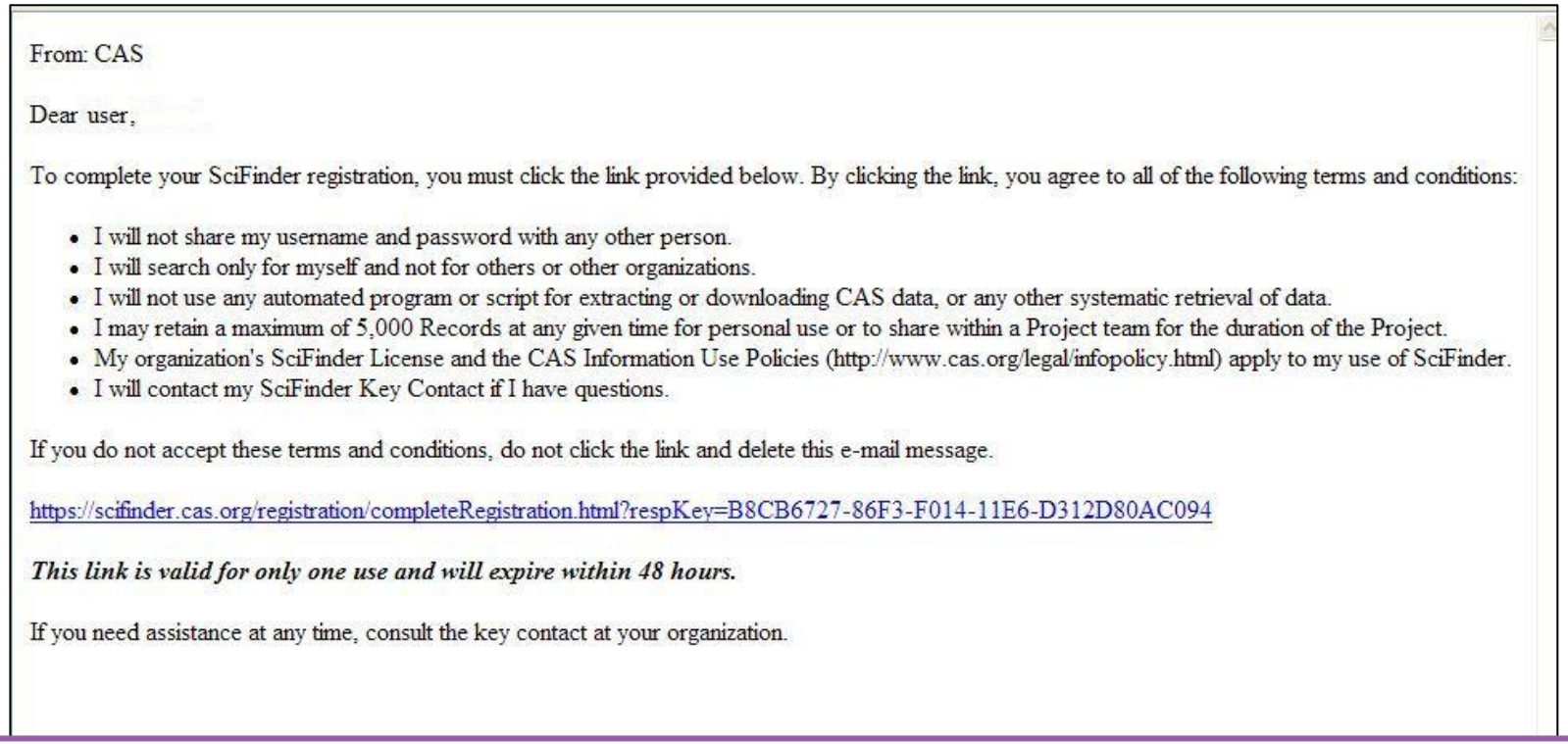

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